Presentation Abstracts

CHEM 23201 - Tuesday

Fall 2012
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Biological weapons, such as anthrax, are treated with Ciprofloxacin—an antibiotic that commonly treats infections. Studying Ciprofloxacin’s operations in the body will identify the attributes that make it an effective antidote to anthrax. Such information can be used to advance the structure of antibiotics and make them more effective. Searching the literature reveals that Ciprofloxacin kills bacteria by binding to its DNA and gyrase enzymes—preventing further duplication. Van der Waals forces drive these reactions. Though basic knowledge of the interaction is known, there is still much to learn about the complete mechanism of ciprofloxacin in the body especially about its ability to bond directly to the bacterial DNA through the use of metal ions.

Pinoresinol is a plant lignan that is found in many common foods and may be useful in disease prevention. In this study, the sources of pinoresinol and its potential medicinal capabilities were examined to see in what ways pinoresinol could benefit health. Researching the literature has provided evidence that lignans, specifically pinoresinol, can improve overall health in humans. Pinoresinol is highly successful at reducing inflammation and has a high degree of conversion into ‘enterolignans.’ These attributes assist in giving pinoresinol a protective effect against cancer and other diseases. The results of this study raise the further questions of what causes the differences in health benefits among lignans, and how enterolignans are more physiologically active than lignans.

I am investigating pentetic acid’s role in chelating metals, since it is a widely used interfering compound for interacting with metals. Thus, by studying the structure of pentetic acid, I will be able to study its mechanism when it interacts with metals. Using multiple scientific databases, I researched the literature. I found that pentetic acid’s conjugate base could potentially form an octadentate ligand. Thus, pentetic acid has a high affinity to chelate metals, since it can bind up to eight bonds around a metal. This property of DTPA is useful in research and in common products. Researching pentetic acid’s highly useful chelating properties leads to the question on the method of removing DTPA’s interaction with the chelated metal.
Consequences of the Structure of Warfarin as an Anticoagulant

Anticoagulants are used medicinally to reduce and eliminate blood clots and therefore protect patients against cardiac illness. Warfarin is an anticoagulant used specifically to treat thrombosis. My research focused on the similarity of the structure of warfarin to vitamin-K and how this contributes to its overall anticoagulant effects. I searched the available literature online and in print and compiled information on warfarin’s mechanism of action focusing on chemical activity. The 3-substituted aromatic ring in warfarin, similar to that of vitamin-K, hinders the synthesis of various clotting and regulatory factors by inhibiting vitamin-K dependent synthesis. Further research focused on natural substitutes of warfarin and similar drugs having fewer interactions with common ingestions is required to decrease thrombotic activity with lesser effects.

The Contradiction of Capsaicin: An Irritant and Pain Reliever

Sometimes a natural analgesic is desired instead of traditional synthetic analgesics. Capsaicin, from chili peppers, is a natural analgesic and an irritant. The goal is to determine how capsaicin interacts with pain receptors as an irritant and an analgesic, and the applications of capsaicin as an analgesic. After searching the literature, I found that sensory neurons become insensitive to capsaicin after prolonged exposure and are simultaneously desensitized to other painful stimuli relieving pain. This desensitization is attributed to death of the neural receptor or damage to the receptor’s peripheral terminals. Capsaicin is applied topically for many conditions. Exposure of sensory neurons to capsaicin is beneficial in the short-term, however the underlying damage to sensory neurons is alarming and there may be detrimental long-term effects.
Dental caries, more commonly known as a cavity, is a bacterial infection that causes demineralization of hard tissues such as the enamel, dentin, and cementum. Although better prevention methods have been researched and oral care has greatly advanced since the early 20th century, in the world today, cavities are still among the most common diseases. Fermentable carbohydrates, such as fructose, provide the energy necessary for the glycolysis reaction that caries-causing bacteria living in dental plaque tends initiates producing acids. The acids decalcify the fibrous protein of the tooth enamel. Fructose, is a natural sugar found in most foods we consume, like fruit and honey. This acid demineralization process is in equilibrium with saliva and fluoride remineralization. Cavities appear due to the equilibrium shift toward the acid demineralization. Cariology is the study of dental caries. By using biochemical reactions, resent dental research publications, as well as earlier research, this study generates a chemical understanding of caries formation. Through research, the pathway to a cavity is known and is used to continuously improve prevention methods. If cariology research continues to advance at a steady pace, dental caries may no longer be a common infection.

13 November 2012

A stable internal environment is critical for cell survival. The cell’s cholesterol level must be properly maintained as it influences membrane fluidity. My research focused on cholesterol synthesis and how its structure affects the cell membrane. I searched the literature using scientific names for cholesterol to acquire relevant structural and synthesis information, which eliminated unrelated results from a basic web search. I discovered the liver primarily synthesizes cholesterol and the rate is contingent on the amount already present. Its structure affects function and position in the bilayer. The hydroxyl group interacts with the polar region, the tetracyclic ring decreases membrane fluidity, and the methyl group increases lipid interactions. As cholesterol imbalances cause many diseases, future research should focus on how to best regulate these levels.
Aspartame: Is it as Harmful as Some May Claim?

Health scare claims are common in the food market today. Aspartame, a common artificial sweetener, is rumored to cause cancer. Aspartame is a controversial item used in its market, so I will research its chemical effects and risks for humans. Available databases and reliable Internet sources provided research literature for the topic. Aspartame has been tested in rats exposed to high levels of the sweetener, and no decisive data indicated that high dosages cause cancer. Human tests have provided similar results; research is still being investigated to find a link between aspartame and adverse health effects. Aspartame appears to be a safe substance to consume even in high dosages. However, there should be further investigation of the long-term effects of human consumption of aspartame.

Histamine and its Role in Treatment of MS

Approximately 400,000 Americans have multiple sclerosis. Although a cure is not known, the use of histamine to treat this disease is being studied. Histamine, the biological molecule involved in allergic reactions, may be used for treatment. The goal of this research is to determine if histamine plays a role in MS prevention or symptom lessening. By searching the literature, a better understanding of the relationship between histamine and MS is hoped to be obtained. According to the literature, histamine has been shown to reduce the proliferation of a cytokine correlated with brain inflammation and loss of neuronal cells’ myelin sheaths. However, stimulation of the wrong receptors of histamine could be counterproductive. Is there a method to selectively determine which histamine receptors are stimulated?

Structure, Function, and Metabolism of Galactose, and the Effects of Galactosemia

Galactosemia is a potentially fatal disease affecting 1 in 60,000 people globally. Galactose ingestion is lethal for galactosemics, while others ingest galactose regularly. This project investigated the structure, function, and metabolism of galactose, and how galactosemia disrupts this metabolism, by searching the secondary literature. The results show that galactose is a hexose used as metabolic fuel and as a part of the blood-type determining carbohydrate chains. Galactose metabolism proceeds through the Leloir pathway, in which three enzymes (GALK, GALT and GALE) can be mutated, prohibiting further breakdown and making galactose toxic. Future research should determine which genes are mutated in each enzyme, and how these mutations alter the enzymes. Ultimately, research should determine how to work around these mutations to allow for effective galactose metabolism.
20 November 2012

11:00 – 11:12 Erin Lavin  Investigation of the mechanistic, structural, and bioactivity differences between Oxycodone and opiate-related drugs of abuse

The line between therapeutic drug use and drug abuse is often a thin one. Oxycodone is used to treat chronic pain but its illegal derivatives are recreationally abused. Understanding how these derivatives relate to their therapeutic precursors is essential in combatting their potential for abuse. Analysis of the mechanism of action, chemical structure, and bioactivity of oxycodone and its derivatives via the literature revealed similarities in their modes of action. Agonistic activity of µ-receptors, and key metabolic reactions such as N-demethylation and O-demethylation are characteristic of both groups. Therefore, the line between therapeutic drug use and drug abuse appears to be derived from dosage. The next question is how oxycodone can be manipulated in order to curb its potential for abuse while maintaining its analgesic capabilities.

11:13 – 11:25 Maria Moreno  Use of Mannitol for post-operative treatment

Medical technology has improved much in the past years, as a result we now have a plethora of different substances that we use to provide medical treatment and it is sometimes difficult to keep track of the effects and uses of each. Mannitol is one of these drugs. The goal is to determine the use and the effects this drug is supposed to have, and report cases of both negative and positive effects. After searching the literature I found that its use in post-operative treatment is to relieve cranial pressure, however, it has been seen to produce negative side-effects, especially on kidneys. How does mannitol affect the kidneys? Is there a way in which it can be administered without having this consequence?

20 November 2012

12:30 – 12:42 Bryce Jones  Indole synthesis and diversification

The biological prevalence of indoles has led to extensive studies on ways to synthesize indole derivatives. The mechanisms of two classic reactions—the Fischer indole synthesis and the Pictet-Spengler condensation—are discussed to explain the effects of using similar reagent derivatives. It is advantageous for researchers to be able to synthesize many derivatives of indole because small changes in a molecule’s shape can radically change its function. 2’ and 3’ indole derivatives can be directly synthesized via the Fischer indole synthesis. Indole derivatives can be further functionalized by the Pictet-Spengler condensation. The ease of these reactions makes them cornerstones of modern organic synthesis.
Morphine: Pain Reliever or Dangerously Addicting?

Relieving severe pain and potential addiction are two of the outcomes of the use of morphine; this causes doctors to be suspicious of morphine even though it is effective. While morphine has been around since the 1800s, doctors are very cautious about prescribing morphine due to the possibility of addiction. Doctors are also cautious even when addiction is unlikely because there is high demand for morphine on the street by addicts. The goal is to determine why morphine is so effective at dealing with severe pain and why addiction to morphine is such a problem among certain types of people, but not others. This was accomplished by doing an in-depth research project, searching the literature, focusing on the trends of morphine addiction as well as the causes of the addiction. Morphine is being shied away from, even though; it is effective, because of problems in prescribing doses, and the non-inferiority of other opiates. In conclusion, the side effects of morphine do not out way its benefits; whether the substitutes are sufficient considering long term side effects has not been determined.

Melatonin: “Hormone of Darkness”

Millions of college students are plagued by a lack of sleep and drowsiness every day, affecting their attentiveness in the classroom and productivity throughout the day. Information gathered through investigation into literature research using various resources has revealed that melatonin is vital to circadian rhythms through its secretion from the pineal gland as part of the endocrine system. This melatonin release is heavily influenced by light in the surrounding environment, and is most heavily released during the night, causing the drowsiness feeling that precedes sleep. Finding ways to control this release through artificial inducing or suppression processes could lead to improvements in medication for countless individuals suffering from a variety of sleep disorders.
27 November 2012

11:00 – 11:12 Amity Wipson  
The effect of beta-carotene on smokers

Lung cancer is a prevalent disease among smokers. In addition to the danger of cigarettes, consuming large amounts of beta-carotene may increase the risk of lung cancer. Beta-carotene is a source of vitamin A and retinol, which are essential for bone development and vision, respectively. By studying the literature, I will investigate why an excess of this necessary compound, in conjunction with cigarette smoke, leads to disease. It has been suggested that beta-carotene is not an anti-oxidant against the carcinogenic free radicals from smoke, but instead acts as a pro-oxidant when taken in high concentrations. Since there is not unanimous consensus that beta-carotene has this effect with the radicals, I am wondering what further experimentation can be done to prove this.

11:13 – 11:25 Daniel Wright  
Phosgene: From Weapon to Reagent.

War fosters vile creativity, and among its deadly creations, chemical weapons may stand as the most heinous. In particular, phosgene, which found infamy in World War I, devastates the human body. Its effectiveness must surely be rooted in its chemical structure. By investigating the literature, it seems that phosgene causes edema in the lungs due to lipid peroxidation by the formation of in situ radical species, resulting in suffocation. However, because the molecule can react with all four of its atoms, especially towards amines, it serves many purposes in various industrial processes including plastic synthesis. With such utility from a century-old weapon, it seems possible that other deadly compounds may be of some currently unknown beneficial use.

11:26 – 11:38 Katy Anthony  
The Chemistry of a Compound that Saved the World: Synthesis, Characterization, Structure, and Physical Properties of Streptomycin

Tuberculosis was a global and fatal disease until the discovery of streptomycin, an antibiotic, in 1946. This project will examine the synthesis and isolation of streptomycin as well as its structure and physical properties. Literature, both recent and old, will be searched to answer these questions. Streptomycin is isolated from the actinobacterium *Streptomyces griseus*. Since its initial discovery, its chemical mechanism of action has been elucidated, and it has been synthesized in large amounts for use as an antibiotic. Streptomycin has fifteen chiral centers, is soluble in aqueous solvents, and acts as a base due to amine groups. Its crystal structure shows evidence of abundant hydrogen bonding. As antibiotic resistance grows, research utilizing streptomycin will continue to be of vital importance in preventing human death.
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12:30 – 12:42 Katherine Chong

Dopamine is a type of neurotransmitter that allows people to feel happiness and love. The presentation will explore the structural characteristics of dopamine and contain an important reaction concerning it. The two hydroxyl groups on the benzene ring of dopamine make it hydrophilic. Dopamine also has similar chemical properties when compared to 1, 2-benzenediol. Furthermore, dopamine is known as the precursor of norepinephrine. In this reaction, dopamine can be converted into norepinephrine via hydroxylation at an aliphatic carbon. This reaction occurs in the human body, in which an enzyme known as dopamine β-hydroxylase is used.

12:43 – 12:55 Daniel Kwasnieski  
Sarin: An accidental killer

In 1936, the accidental discovery of the nerve agent tabun led to a succession of new developments in organophosphates (OPs) as potent acetylcholinesterase inhibitors, authorized by Nazi Germany. These new compounds came to be known as the G-series, and principal among them was sarin, or GB. This study highlights the synthesis and weaponization of sarin, its inhibitory effect, and agents used to reverse this deadly effect. As of yet, it has been found that sarin can be produced by mixing methylphosphonyl derivatives with isopropyl alcohol, which can be loaded into binary shells used as effective vehicles to deliver sarin to military targets. Furthermore, it acts by binding to a serine residue in acetylcholinesterase and can become irreversibly trapped if reactivating agents called oximes are not quickly administered. However, in vivo studies of oximes have not been thoroughly explored and much remains to be discovered in counteracting sarin.

12:56 – 1:08 Elizabeth Tso  
Caffeine: The Competitive Inhibitor

Caffeine is consumed by 90% of Americans on a daily basis. As the main ingredient in energy drinks, it’s known to prevent sleep and increase endurance. By examining Caffeine’s structure and properties, we can understand how nerve cells confuse it with adenosine, a neurotransmitter that triggers sleep. Since caffeine is both water and lipid soluble, it can easily cross the blood-brain barrier. Once inside, it is capable of binding to adenosine receptors due to its structure being similar to that of adenosine. Caffeine binds to the adenosine receptors A1 and A2A but produces the opposite result of adenosine by increasing heart rate and thus results in a rise of adrenaline causing us to believe we have more “energy.”
Many biological and chemical experiments rely on indicators or colored markers to see how a process or reaction is progressing. One example of such a colored indicator is bromophenol blue (BPB). This study examined the structure and physical properties of BPB to help explain why bromophenol blue is used as an acid-base indicator in experiments. By searching the literature, it was found that BPB is a good indicator because the protonated and deprotonated forms of the compound can absorb different wavelengths of light, therefore taking on different colors. The structure of BPB is very similar to other indicators, and it would be interesting to see if the compound could be changed to work in other pH ranges.

Attention-deficit Hyperactivity-Disorder is a neurobehavioral disorder that negatively affects millions by decreasing their ability to focus. One primary cause of ADHD is irregularity in the function of neurotransmitters like norepinephrine, which causes problems by binding improperly to adrenergic receptors. The goal is to learn how norepinephrine binds incorrectly to receptors, what effect those chemical changes have on the brain, and how these changes manifest as ADHD symptoms. Information will be gathered through researching the chemical literature. Results showed that improper binding of norepinephrine causes early signal termination or degradation of the neurotransmitter into other molecules. Inattention resulted from norepinephrine levels being too low to sufficiently stimulate the brain. There is still a question as to what chemically causes abnormal norepinephrine behavior.

While many organically derived compounds have medical uses, nerolidol seems to be simply a flavoring agent. Does nerolidol have any medical uses that are being overlooked or is it simply a flavoring agent? This question was answered by searching chemical and medical databases for any information on medical uses of nerolidol. It was found that nerolidol is not a major player in the medical field, but is being tested as a skin penetration enhancer for epidural injections. There may be yet undiscovered medical uses for nerolidol, but they have not been explored because they are not yet necessary in the present day. It does not seem, however, that the scent itself has been tested as some sort of repellent, which would be interesting.
Today’s scientists have worked non-stop to develop cures for various cancers that constitute a deadly, fast-growing epidemic in the world. Surprisingly, it was discovered that Benzaldehyde, a simple molecule found in apples and almonds, has significant cancer-fighting abilities. This presentation explicates these abilities and compares them to Benzaldehyde’s other qualities and characteristics. Much of the information was found from review and journal articles as well as from library reference material. Research and resources show that a gluconated form of Benzaldehyde (called BG) caused an "overall objective response rate" of mice to cancer. Other research shows that Benzaldehyde has been successful in treating carcinomas. Such findings lead to the proposal of why Benzaldehyde is not more commonly constructed and utilized by Pharmaceutical Companies and doctors.