

Presentation Abstracts

CHEM 23202 – 01

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25 March 2008

12:30 – 12:42 Catherine Cassou Lycopene

It is essential to ascertain efficient modes of isolation, preparation, and identification of lycopene, which has been identified as a reducer of prostate cancer risk due to its antioxidant properties. Through investigating the literature, I discovered that lycopene is easily extracted from produce such as spinach by HPLC. Lycopene can also be synthesized from pseudoionone by McMurry coupling or from bacteria, even bacteria that do not naturally synthesize carotenoids, via metabolic engineering. Furthermore, lycopene is readily identified through UV-Vis, proton and carbon NMR, IR, and MS spectra. Progress in the science behind lycopene and its synthesis could lead to a lowering of prostate cancer rates as this compound becomes more influential in medicine.

12:43 – 12:55 Conor McLaughlin Astaxanthin

Astaxanthin is a naturally occurring red pigment found in many biological species including shrimp, lobster, and salmon and has been ascribed as an exceptional antioxidant in the cell. Astaxanthin belongs to the family of carotenoids known as xanthophylls and is produced principally by plants and microalgae. Recent interest in the antioxidant activity of astaxanthin in the cell has led to proposed roles for astaxanthin in various therapeutic applications. Through a thorough analysis of the primary and secondary literature, further details concerning the synthesis, characterization, and role astaxanthin plays in the cell were investigated. This research led to insight concerning the preferred laboratory synthesis of astaxanthin via a double Wittig reaction. Physical properties, including spectral data, were explored in an attempt to elucidate how its structure and chemistry helps confer utility to the cell. The antioxidant activity of astaxanthin, especially with respect to its singlet oxygen quenching and radical scavenging capabilities, was also explored allowing for a better understanding of recent studies in which astaxanthin was shown to reduce essential hypertension.

1 April 2008

12:30 – 12:42 Tyler Hulett

As a person ages there is the potential for them to become intolerant to lactose; they cannot digest it as they did in infancy. To understand intolerance, as well as the eventual dietary symptoms that accompany it, it is necessary to understand how lactose is normally digested into its monosaccharide components. The answer to this question is readily available through analysis of print and electronic literature. The digestion of lactose in mammals, humans included, requires the presence of the lactase enzyme. People that have lost the ability to produce lactase can no longer digest lactose to glucose and galactose, thus becoming intolerant. Bacteria in the intestines flourish on the undigested sugar, resulting in the uncomfortable symptoms associated with lactose intolerance.

12:43 – 12:55 Amy Liesenfelt Fructose: A Sweet Way to Health Problems

Fructose is a compound used as a sweetener in many foods such as corn starch and soda, and found naturally occurring in honey and fruit. There are many derivatives of fructose and I will be examining the D-fructose form. The consumption of fructose has potentially harmful health implications that may affect uric acid, LDL levels, obesity, hyperactivity, tooth decay, and insulin resistance. Literature research of the structure, synthesis, and commercial uses of fructose was used to gauge the compound's health risks. There is still debate about whether to recommend fructose for diets when it has such harmful effects. The magnitude of the health risks resulting from fructose intake must be assessed in order to develop possible cures and have preventative programs implemented.

12:56 – 1:08 Mike Purcell Production and Commercial Use of Glucose

Glucose is an energy source used in almost all organisms on the planet. In order to gain a more complete understanding of this important compound, an inquest into modes of synthesis, chemical properties, and the commercial use of glucose in controlling DNA recombinant protein production in *E. coli* was made. This was accomplished by reviewing the scientific literature. Results show that upon decreasing glucose concentrations in cell cultures, the number of *E. coli* in the culture stays constant, preventing environmental stress. The studies show that protein production can still be accomplished under glucose starved conditions, while keeping environmental stress to a minimum.

1:09 – 1:21 Bert Williams Sucrose and its Effects on Humankind

Sucrose is a naturally occurring sugar that is present in many foods people eat everyday. Because of its prevalence, it is important to determine the structural significance, modes of synthesis, and its biochemical effects on humans. Through the consultation of primary and secondary literature, the structure, synthetic processes, and biological effects of sucrose were studied. Animal studies have linked the consumption of sucrose with insulin resistance, memory deficits, and tumor growth. Sucrose has the highest purity of any organic substance synthesized on the industrial scale (>99% pure). A current, non-food application of sucrose is in biofuels. Because of sucrose's numerous applications, it is an extremely important compound to study. Biologically, it has impacted humans and its diversity in applications could make an even bigger impact.

8 April 2008

12:30 – 12:42 Molly Smith Neotame: Sweeter than sugar

A derivative of aspartame, neotame is a high-potency sugar substitute, reportedly 6000 to 10000 times sweeter than sucrose. First synthesized in 2000 by the Nutrasweet Company and approved by the FDA in 2002, neotame's similarities to aspartame, the popular commercial sweetener, have bred controversy over possible health risks. Currently, neotame appears in few commercial goods. Does neotame pose the same carcinogenic threats as aspartame? By reading the chemical literature and health reports on sugar substitutes, not much is known about the long-term affects of neotame, though the amount needed to sweeten is far less than that of aspartame. Further studies are needed to determine the affect of neotame in biological systems, as well as the broader health effects of non-caloric sweeteners in modern diets.

12:43 – 12:55 Joseph Maciuba The Synthesis, Classification and Metabolism of Aspartame

Aspartame is an artificial sweetener found in over 6,000 products. Over 200 million people ingest it as a sugar substitute. It is important to know how aspartame is synthesized and characterized since it is found in many products. If health problems accompany the use of aspartame, this could have a negative effect on the population. Analysis of literature will explain the creation and characterization of aspartame and how it is metabolized. It is synthesized through the reaction of phenylalanine and aspartic acid, forming a compound 200 times sweeter than sugar. There has not been a conclusive study found that definitively links aspartame to the cause of harmful effects in the body, and thus more long term research must be conducted on aspartame.

12:56 – 1:08 Mark Brickey Saccharin: Risk assessment and synthesis of an artificial sweetener

Saccharin is consumed by millions of people as a non-nutritive sweetener. It has 200-700 times the sweetening power of granulated sugar and has been shown to cause occurrences of bladder cancer in rats. This study will investigate the potential hazardous effects of consuming large amounts (5 mg/kg/day) of saccharin, those effects on future generations, characterization of saccharin found in common diets as well as the synthesis of saccharin. Investigating current studies, animal bioassays, and epidemiological studies has led to several conclusions. It is experimentally proven that saccharin in large doses does lead to a higher inclination of bladder cancer in rats. Although this has not been witnessed in human beings, there is still a possibility that saccharin can pose as a carcinogenic substance to humans.

1:09 – 1:21 Michelle Hackner Sucralose: Synthesis, Characterization, and Safety

Sucralose is one of the most widely used artificial sweeteners in America. It currently holds a 62% market share and is found in more than 4,500 products. Sucralose has been celebrated as a healthy alternative to sucrose; however, concerns remain about possible health risks associated with the compound. These concerns can be better understood when the structure, synthesis, and chemical reactivity of the compound are better understood. For this study, literature about the development and production of the compound, its characterization, and recent studies on its health effects were examined. After reviewing the literature, it was found that while more than 100 scientific studies have been conducted on the safety of sucralose, sucralose has not been proven to have any adverse effects on human health.

15 April 2008

12:30 – 12:42 Alison Schilling The genetic disorder Trimethylaminuria and the breakdown of the FMO3 gene in metabolizing Trimethylamine to its N-oxide

The inability of organisms to metabolize trimethylamine (TMA) into its N-oxide results in the trimethylaminuria, a genetic disorder that affects 1 in every 10,000 people. To obtain a greater understanding of this disorder, trimethylamine was synthesized and an analysis was done using spectral data and knowledge of the general physical properties to understand the difference between TMA and its N-oxide. Trimethylaminuria results from the mutation of the FMO3 gene on chromosome 1, which makes an enzyme that metabolizes nitrogen-containing compounds. If both copies of the gene are mutated, the individual will be unable to metabolized trimethylamine into the odorless N-oxide, resulting in a fishy odor. Those afflicted with trimethylaminuria can live normally if they maintain a strict diet low in trimethylamine.

12:43 – 12:55 Kelly Marszalek

Cadaverine: When good eggs go bad

After death, the human body is a site for countless chemical reactions. One of such is the production of cadaverine, a compound that creates the “rotting eggs” smell in corpses. This project’s goal was to locate data that describes the synthesis of and characterizes cadaverine. Using the Notre Dame Library system and the internet, it was found that cadaverine is created by the decarboxylation of lysine by *Escherichia coli* and *Clostridium bifermentans*. The smell of cadaverine is typically an indicator that something is amiss in the body. When a person is alive, the smell can signify infection, such as vaginosis. When dead, it can aid in murder investigations. Although rancid, cadaverine is an important chemical that helps indicate when the normalities of life are interrupted.

12:56 – 1:08 Lauren Schilling

Indole is an organic compound of a benzene ring fused to a five membered pyrrole ring containing nitrogen. It is present in a large number of naturally occurring compounds including, the plant growth hormone indole-3-acetic acid, the animal tissue serotonin, and the pigment indigo. After searching the literature, it was found that Indole is synthesized in different ways. The most popular are the Leimgruber-Batcho and the Fischer Indole synthesis. Having the ability to artificially synthesize Indole allows it to be used widely. Main uses of Indole are its presence in coal tar and artificial sweetener. An interesting thing about Indole is its presence in high quality perfumes, despite its harsh fecal smell. It is also currently being studied as an anti-carcinogenic compound.

1:09 – 1:21 Sarah Matthys

Pyridine: The Compound that Doesn’t Rest

Pyridine is a heteroaromatic compound with properties that have been exploited in industrial chemistry. Since pyridine is widely used in synthetic reactions, understanding its chemical properties is pivotal to understanding and developing more efficient syntheses. The purpose of this study is to determine the chemical properties that make pyridine useful. After searching the literature and analyzing spectra, it was determined that reactivity of pyridine is dependent on heteroaromaticity. The aromaticity of pyridine makes it a stable solvent, the heteroatom increases the polarity, and the electron lone pair on nitrogen makes it nucleophilic. The literature also indicated that pyridine is a hazardous compound and must be used with care. Therefore, future research should be directed toward developing compounds that have pyridine’s nucleophilic, heteroaromatic properties without the hazards.

22 April 2008

12:30 – 12:42 Lamarr Holland Stability of avobenzone (butyl methoxydibenzoylmethane) in UV-A light over extended periods of time.

The ability of the molecule avobenzone (butyl methoxydibenzoylmethane) to absorb UV-A rays suggests that it would be an effective ingredient in sunscreen products. However, because of its tendency to breakdown in light, it has been shown to provide limited protection over time. The compound is synthesized from a claisen condensation involving hydrochloric acid with sodium amide. Research concerning the properties and patterns of behavior of avobenzone was compiled and analyzed to investigate the issue. From this it was uncovered that avobenzone does have a tendency to degrade under constant exposure to UV-A light, but in combination with other chemicals such as titanium dioxide can provide adequate protection. This use of avobenzone could supply protection from UV-A light.

12:43 – 12:55 Alex Dzunik Oxybenzone: Sun Block or Health Hazard?

Oxybenzone is a chemical compound that is an active ingredient in most common sunblocks. Oxybenzone is synthesized using an alkyl aryl ether and di-Me carbonate. It acts as an excellent ultraviolet light blocker, which has a low occurrence of side effects in comparison to other UVA blockers. However, there are still worries as to the dangers of the prolonged use of oxybenzone. Some people develop a photoallergy after extended use. Another serious concern is that oxybenzone can be rapidly photo-oxidized into a by-product, which suppress antioxidant systems. To explain these risks and possible solutions to them, I will present the results and explanations of various experiments scientists have conducting concerning the health risks, with a multitude of approaches, including spectroscopy and various phototesting techniques to analyze oxybenzone and it's role in UV protection. Studies have shown that oxybenzone does indeed exhibit the side effects mentioned, and has the possibility of developing photoallergies in a small portion of the population. However, the studies have indicated that while these problems exist, the rate of occurrence is quite small, not enough for a serious health concern, and significantly safer than other comparable UV blockers. The conclusion that these results show is that oxybenzone, while not perfect, is the safest of the current generation UV blockers.

12:56 – 1:08 Marissa Collard Protecting Our Skin: Octyl Methoxycinnamate

Skin protection is important to prevent skin cancer and other skin diseases. Octyl methoxycinnamate is a common component of sunscreen because of its ability to absorb UV rays, thereby giving good protection against harmful sun rays. There are several different syntheses of octyl methoxycinnamate, but this report will focus on one of the most efficient. Characterization of this compound including boiling point and density will also be discussed. The UV blocking properties of octyl methoxycinnamate are of interest, since there are some unwanted side effects and overexposure could lead to more problems. Many recent journal articles have cited certain groups of people to be more susceptible to such side effects.

1:09 – 1:21 Will Culligan Para-aminobenzoic acid as a sunscreen agent

Para-aminobenzoic acid (PABA) is a UV filter commonly used in commercial sunscreens. PABA is FDA-approved as an active ingredient in sunscreens, and is historically a popular choice as a UV filter, but recent competition from other compounds, including PABA derivatives, has emerged due to reports of harmful dermatological side effects. The chemical properties of PABA are well documented, and several effective syntheses exist. PABA's efficiency as a sunscreen has also been tested. In this study, the literature was searched for information on PABA, specifically relating to sunscreens. PABA shows chemical and spectral data consistent with its structure, and is an effective UV filter, but harmful side effects have been documented. While these are not conclusive, currently other compounds are favored over PABA as active ingredients in sunscreens.

29 April 2008

12:30 – 12:42 Chris Schaal

Lutein, a xanthophyll and known antioxidant, is implicated in the treatment of Age-Related Macular Degeneration (AMD), the leading cause of vision loss in the United States. Found in many green, leafy vegetables, it is one of the most common pigments in the natural world. In this review, Lutein's commercial and biological synthesis will be discussed. Spectral characteristics will be described, as well as the potential uses for Lutein in the medical realm. Examination of current research suggests that while increased Lutein in the diet shows some promise in preventing and treating AMD, these results are best accomplished by a "cocktail" of different carotenoids and antioxidants. Lutein's role in the body is complex, and further study is needed to improve AMD treatment through carotenoid supplementation.