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ZINC(II) AND NICKEL(II) COMPLEXES THAT DEMONSTRATE DNA SELECTIVITY: POTENTIAL QUADRUPLEX DNA BINDERS

A series of small zinc (II) and nickel (II) complexes have been synthesized and characterized, and these complexes have shown sensitivity towards different forms of DNA. The fluorescence enhancement or quenching of these complexes was used as markers for sensitivity. The fluorescence emission of each complex was monitored as a function of DNA concentration. The changes to the emission intensity were observed when the double-stranded quadruplex G4T4G4 (12mer), and the human telomeric DNA sequence, AGGG(TTAGGG), (22mer) were added in the 5-30 ppm range to the two neutral octahedral complexes. Both of the quadruplex DNA molecules and the duplex calf thymus DNA showed interaction towards a cationic square-pyramidal complex. Depending on the fluorescence trend, Stern-Volmer and a modified Wolfe’s analysis were used to determine binding constants, which were on the order of 10^6-10^8 M⁻¹.

EFFECT OF HALOGEN SUBSTITUTION ON THERMAL DECOMPOSITION OF METHYL AZIDE

Methyl azide (azidomethane, CH₃N₃) is an energetic compound whose thermal decomposition pathway involves the reaction CH₃N₃ + CH₃=NH + N₂, with the release of significant amounts of energy. The reaction involves the dissociation of an N-N bond in concert with a 1,2-hydrogen shift. In the current study, methyl azide is compared with its difluoro and dichloro counterparts to determine the effect of halogen substitution on the energetic properties of the molecules. Theoretical calculations are carried out to determine both reaction barriers and energy release for the dissociation reaction. Density functional theory and coupled-cluster theory are used in this study. Trends with respect to halogen substitution and basis set effects are calculated and discussed.

ADDITIVE-FREE SYNTHESIS OF MONODISPERSED GOLD NANOPARTICLES WITH CYCLODEXTRINS

Gold nanoparticles (AuNPs) are very useful for various applications in the biomedical field. In this study we demonstrate a new method to prepare AuNPs yielding reproducible particle sizes solely using a-, b-, or g-cyclodextrin, which serve as both reducing and dispersing agents. These biomolecules constitute excellent ligands that improve the water solubility, bioavailability, and stability of hydrophobic molecules for delivery applications. In contrast to previous methods, our synthesis produces monodispersed AuNPs without using harsh reagents or additives. Therefore, the resulting AuNP solutions are more suitable for in vitro and in vivo applications.

IDENTIFYING ANTI-CANCER STRUCTURAL FEATURES/PATTERNS AMONG GINSENOSIDE STRUCTURAL ANALOGS USING A UNIQUE APPROACH IN CHEMICAL EDUCATION AND STATISTICAL ASSESSMENT

In this project, Undergraduate chemistry research students worked together to develop a new process for identifying specific anti-cancer structural features among a large subset of natural structural analogs of the ginsenoside compound. Ginsenoside has been found to be a bioactive compound in the Herbal Medicine, Ginseng. Although the structure-based anti-cancer molecular mechanism of action is still largely unknown, a large database of structural analogs of the ginsenoside compound exists and continues to expand (see PubChem). In order to identify patterns in structural features consistent with anti-cancer bioactivities among the compounds in the PubChem database, the research team developed new assessment approaches. The process involved triangulating research methods from the sub disciplines of Chemical Education, Computational Chemistry and Statistical Assessment. Results from this study allowed for identification of a statistically significant anti-cancer structural feature among a relatively large set of ginsenoside analogs. In addition, the research lead to the development of assessment processes that can be applied to other natural analog compounds with medicinal potential.

A RELIABLE METHOD TO MEASURE THE MELTING TEMPERATURES OF DNA OLIGONUCLEOTIDE TRIPLEXES

The formation of DNA triplex structures has attracted much interest because it provides a useful approach to recognize DNA duplex in a sequence specific manner. The thermal stability of triplex DNA is normally determined using thermal denaturation monitored by UV spectroscopy. Under physiological conditions, the melting temperatures of DNA oligonucleotide triplexes are often lower than room temperature; therefore, it is difficult to obtain reliable melting curves due to moisture condensation on the surface of cuvettes if no constant airflow is available for the UV instrument in the lab. In this paper, we report a reliable method to measure thermal denaturation of DNA oligonucleotide triplexes that dissociate below ambient temperature with airflow supplied by a portable air compressor. With the method, we investigated the melting of a DNA oligonucleotide triplex (22-mer TAT) at various salt concentrations and determined salt concentrations suitable for studying ligand-DNA oligonucleotide triplex interactions. This method is cost effective and can be readily set up in a biochemistry lab not equipped with a built-in air/nitrogen supply system.

STATISTICAL ASSESSMENT USING A UNIQUE APPROACH IN CHEMICAL EDUCATION AND PATTERNS AMONG GINSENOSIDE STRUCTURAL ANALOGS IDENTIFYING ANTI-CANCER STRUCTURAL FEATURES/
RECYCLING WASTE VEGETABLE OIL AND SEASHELLS FOR BIODIESEL PRODUCTION

The price of raw materials and the chemical processing associated with the current wide scale method of biodiesel production pose significant financial and environmental costs. Waste vegetable oil and waste seashells can serve as more sustainable sources of the feedstock and catalyst needed to produce biodiesel, and are more favorable than the common use of edible vegetable oils and the homogeneous catalyst KOH. The food industry annually produces millions of pounds of waste vegetable oil and waste seashells; thus, the repurposing of these materials in biodiesel production could offset the cost of their disposal. The heterogeneous catalyst CaO was produced from calcined waste mussel shells and successfully catalyzed the transesterification of waste vegetable oil to produce fatty acid methyl esters (FAMEs), or biodiesel. X-ray Powder Diffraction (XRD) confirmed the conversion of raw waste mussel shells to CaO, and 1H NMR and FTIR were used to analyze the conversion of the feedstock to biodiesel. CaO sourced from waste mussel shells was shown to be a competitive alternative to KOH for the transesterification of waste vegetable oil to produce biodiesel.

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INVESTIGATION INTO ANTICANCER PROPERTIES OF HAOUAMINES BY COMPUTATIONAL DOCKING TO TUBULIN, TOPOISOMERASE II, AND SMOOTHENED

Alkaloids haouamine A and atrop-haouamine A have been shown to exhibit high activity against human colon and prostate cancer cells, though the mechanism for cytotoxicity remains unknown. In the present study, cancer inhibition by haouamines was investigated using computational methods, with optimization of ligand geometry by HyperChem® followed by docking with AutoDock™ Vina to target receptors. β-Tubulin, topoisomerase II, and Smoothened were selected as receptors because they are implicated in many forms of cancer, including colorectal cancers. Docking of the haouamines to these receptors was compared to binding of known anticancer compounds, including vincal alkaloids, anthracyclines, and cycloamine which are known to target tubulin, topII and Smo, respectively. The tubulin binding sites for haouamine A and atrop-haouamine A determined in silico mimic those of vincal alkaloid inhibitors whereas haouamine B, which is ineffective as a cancer inhibitor, does not bind at the same sites. Docking of the haouamines to topII indicated binding in close proximity to the catalytic DNA replication site, which is also where known anthracycline inhibitors bind. Again, the binding of haouamine B showed significant differences. Binding of all haouamines to Smo did not reveal any similarities to the known Smo inhibitor, cycloamine. The results relate to how haouamine A and its atropisomer inhibit cancers.

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BIOCONVERSION OF BUTANAL AND 13C ACETALDEHYDE CONVERSION IN THREE CHARACTERISTIC STRAINS OF SACCHAROMYCES CEREVISIAE

The primary purpose of this research was to analyze the effectiveness of using common Saccharomyces cerevisiae yeast strains to convert butanal into butanol. Butanol can be useful in the generation of biofuels. Additionally, the advantage of using butanol in fuel blends as opposed to ethanol is the higher energy content of butanol. We studied butanal bioconversion in Baker’s yeast, top fermenting Ale yeast and bottom fermenting Lager yeast. Lager yeast did not produce any additional alcohol while Baker’s yeast produced the most alcohol on a per gram basis. Ale yeast was moderate in production of alcohol. We also used NMR spectroscopy to study the propensity of these strains to convert 13C acetaldehyde to 13C ethanol based on relative peak integrals of 13C ethanol and 13C DMSO. Next generation studies will further define the tolerance of Baker’s and Ale yeast to butanal concentrations and their ability to metabolize other aldehydes.

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DESIGNING TARTRATE BASED PHASE TRANSFER CATALYSTS FOR ASYMMETRIC REDUCTIONS USING SODIUM BOROHYDRIDE

A systemic study of how changing the groups on a tartrate-based diammonium salt affected the asymmetric induction during the reduction of acetophenone. Unlike previous reports, the asymmetric reduction involved systems that were dependent on how well the borohydride anion interacted with the active binding site of the ammonium salt. The diammonium salts were prepared using appendages of different sizes and polarity to see what effect that had on the stereochemical outcome of the reduction. Based on the results of the initial reactions, a new class of crown ether that contains a quaternary ammonium salt unit as one of the heteroatoms on the crown ether was proposed and prepared. This new catalyst yielded a significant increase in the asymmetric induction of the process.

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