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ISOLATION OF ADENOCHROME FROM THE BRANCHIAL HEARTS OF THE COMMON BROWN OCTOPUS

Adenochrome is an iron-binding metalloprotein concentrated in the two branchial hearts of the common brown octopus, *Octopus vulgaris*. It was first described in 1942, however, its structure and physiological function have yet to be determined. The last attempt to deduce the structure was published in 1979 and was based on the iron free form of the material termed desferriadenochrome. This study contained mixed results which could be due to the harsh purification procedure utilized. Adenochrome is known to have a high affinity for Fe (III) and therefore has potential as an iron chelation therapy drug. Desferal®, the current treatment for iron overload, has several negative aspects such as an exorbitant price and a painful delivery procedure similar to kidney dialysis. The search for novel iron complexing agents has therefore intensified, resulting in this investigation of adenochrome. For the first time, adenochrome has been isolated in its iron bound form and deemed pure by sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE) and high performance liquid chromatography (HPLC). Electron paramagnetic resonance, infrared and ultraviolet-visible spectroscopy indicate the presence of a single ferric ion coordinated by oxygen ligands.

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A MOLECULAR INFORMATICS ANALYSIS OF A κ OPIOID RECEPTOR MODEL AND TWO LIGANDS

A plausible κ opioid receptor model was analyzed using two compounds known to interact with the active site of the protein. Extension of the docking box demonstrated that the κ opioid receptor contained at least two distinct binding locations within the active site.

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SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF A NOVEL TRIS-INDOLYL AMINE

A first-generation tris-indolyl amine has been designed and synthesized based on the tripodal framework of the TRENSOX compounds. The structure of the tris-indolyl amine, derived from X-ray crystallography, reveals that the molecule has a folded conformation stabilized by traditional and weak H-bonds and π-π interactions between the indole moieties of the arms of the tripodal system. An electrostatic potential surface calculation on one arm of the amine suggests that electrostatics play a role in establishing the folded conformation.

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AN AB INITIO STUDY OF INTERMOLECULAR INTERACTIONS OF GLYCINE, ALANINE AND VALINE DIPEPTIDE-FORMALDEHYDE DIMERS

Ab Initio calculations were performed on glycine, alanine and valine dipeptide-formaldehyde dimer systems. It was found that as the R-group of the amino acid dipeptide increases in size, the interaction energy remains fairly constant due to the stabilization effects of the hydrogen bonding in each dimer system. Such information is valuable to explain the prominence and structural properties of glycine, alanine and valine in globular proteins.

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AN ANALYSIS OF ENVIRONMENTAL FACTORS MODULATING FIBRILLATION OF A SMALL NEURO-PROTEIN α-SYNUCLEIN

Lewy bodies and Lewy neurites are pathological hallmarks of several neurodegenerative disorders, such as Parkinson's and Alzheimer's diseases, and Dementia with Lewy Bodies, to name just three. These polymerized and highly stable inclusions, being found in the mid-brain, are predominantly comprised of a small neuroprotein, α-synuclein. α-Synuclein belongs to a group of natively unfolded proteins, which have been shown to have little or no ordered structure under physiological conditions. The mechanism for the conversion from an unfolded protein to highly folded polymer has yet to

be determined. The protein's fibril form renders it inactive to the physiological processes in which it is normally involved. Examinations are currently analyzing the rate, cause, and mechanism of fibrillation. It has been shown that environmental factors promote fibril production; these factors include, but are not limited to pH, temperature, metal cations, pesticides, polycations and polyanions, membrane surface, etc. We are showing here that anions represent another factor that has a direct effect on the ability for α-synuclein to undergo fibrillation.

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CALIX[6]ARENE DERIVATIVES SHOW GAS-PHASE COMPLEXATION OF AMINO ACIDS IN ELECTROSPRAY IONIZATION MASS SPECTROMETRY (ESI-MS)

Non-covalent inclusion complexes formed between amino acids and derivatized calix[6]arenes were observed in electrospray mass spectrometry. The ester derivative **6** and the amide derivative **8** of calix[6]arene yielded protonated amino acid complexes in the gas-phase. The complexes $[M:AA+H]^+$ were observed for some of the 20 amino acids in MS analysis. Only the amino acids arginine, histidine, lysine, cysteine, and valine formed stable adducts. The dissociation behavior of the complex between protonated histidine and the calixarene ester **6** and the calixarene amide **8** under low-energy collision-induced dissociation (CID) conditions was studied. Different qualitative proton-affinities were observed. This may prove helpful in correlating known gas-phase basicities of amines with calixarene complex strengths measured by CID.

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FUEL INSTABILITY AND THE CONCENTRATION OF ORGANO NITROGEN COMPOUNDS IN A MIDDLE DISTILLATE FUEL FROM THAILAND

Decreasing crude oil supplies has lead to the import and use of foreign fuels. Middle distillate fuels are used for ground, water, and air transportation purposes. It is thus important to study the chemical composition of foreign fuels to elucidate the quality of middle distillate fuels in terms of fuel instability. Instability and incompatibility are terms that denote fuel degradation. Reaction mechanisms leading to fuel degradation are difficult to identify. Results from our laboratory indicate that organo-nitrogen compounds are active participants in this sedimentation process. Middle distillate fuel from Thailand purported to form sediment and thus be unstable was analyzed.

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SYNTHESIS OF A SERIES OF ISATIN-3-THIOSEMICARBAZONE-5-SULFONIC ACID COMPOUNDS AND STRUCTURAL CHARACTERIZATION USING NMR SPECTROSCOPY

Interest in compounds related to 1-methylisatin thiosemicarbazone is based on its antiviral activity. This work will present the synthesis of a series of isatin-based monothiosemicarbazone compounds. The isatin-5-sulfonic acid substrate was reacted with thiosemicarbazide, 4-methyl-3-thiosemicarbazide, 4-phenyl-3-thiosemicarbazide, and 4,4-dimethyl-3-thiosemicarbazide to give a series of four monothiosemicarbazones. The sodium salts of the following compounds were characterized by ^{1}H NMR, ^{13}C NMR, IR, and UV-VIS spectroscopy: isatin-3-thiosemicarbazone-5-sulfonic acid, isatin-3-methylthiosemicarbazone sulfonic acid, isatin-3-phenylthiosemicarbazone 5-sulfonic acid, and isatin-3-dimethylthiosemicarbazone 5-sulfonic acid. The compound acenaphthenequinone dimethylthio-semicarbazone was also synthesized for comparison. The data supports an assignment for the structure of the isatin thiosemicarbazones to include a stable and strongly hydrogen-bonded hydrazinic proton that forms a portion of a uniquely characteristic six-membered ring. The far-downfield resonance (12-14 ppm) in the proton NMR spectrum for this unique hydrogen-bonded proton makes it very easy to identify, and the position of this resonance is dependent upon ring strain factors.

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