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LEAD UPTAKE BY *SOLIDAGO RUGOSA* AND *SPIREA LATIFOLIA*

The uptake of lead from soil by *Spirea latifolia* (Meadowsweet) and *Solidago rugosa* (Golden Rod) was examined. Both species showed a time dependent accumulation of lead in their tissues when grown in soil with elevated lead levels. The concentration of lead in the leaves of the *S. latifolia* was 19.2, 49.8, and 96.3 µg lead/g dry weight plant at 8, 23, and 27 weeks, respectively. The controls plants had 5.0, 27.3, and 29.4 µg lead/g dry weight of plant at the same intervals. Similar accumulations and trends were seen in the stems and roots. The differences were all significant at the 99% level (student's t test). The concentration of lead in the *S. rugosa* leaves was 93.2 and 108.7 3 µg Lead/g dry weight plant at 24 and 28 weeks. The controls had 27.4 and 31.5 µg Lead/g dry weight of plant respectfully. These differences were significant at the 95% level.

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ISOLATION AND PURIFICATION OF QUERCETIN 2,3-DIOXYGENASE FROM *ASPERGILLUS FLAVUS* VIA LECTIN AFFINITY CHROMATOGRAPHY

Quercetinase is an enzyme excreted by the mold, *Aspergillus flavus* when grown on rutin. Characterization of the enzyme involves first isolating and purifying the enzyme from media in which *A. flavus* has been grown. Improved techniques for this isolation are presented using methods including lectin affinity chromatography and capillary electrophoresis. A pure sample of quercetinase has been obtained and found to have $K_m = 3.5 \times 10^{-6}$M.

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THE ANALYSIS OF NICKEL AND COBALT BY FLOW INJECTION ANALYSIS USING PAR, 4-(2-PYRIDYLAZO)-RESORCINOL, AND TRITON X-100

A flow injection analysis, FIA, method for the determination of cobalt(II) and nickel(II) using PAR and Triton X-100 has been developed at a lower pH and without EDTA than previously reported. The surfactant method that has been developed eliminates the hot water bath and fifteen minute waiting period in the case of cobalt and the two five minute waiting periods in the case of nickel. The new methods formed a Beer's Law calibration plot at 510 nm with manual spectrophotometric analysis with a molar absorptivity that was 9% below the more time consuming PAR method of cobalt and had an increased sensitivity of 5% for the nickel determinations. The FIA system employed a 10 µL sample loop, a 4.5 m reaction coil, 2.00 mL/min flow rate the two metals had linear response between 0.25 to 3.00 ppm with a correlation coefficient of 0.993 for cobalt and 0.990 for nickel. The surfactants sodium dodecyl sulfate and cetyl pyridinium chloride were also investigated.

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AN INVESTIGATION OF THE ENERGETICS OF BINDING SMALL INORGANIC COMPLEXES TO DNA

The binding of the anti-tumor drug cisplatin [*cis*-diamminedichloroplatiunum(II)] to DNA has modeled using the computer modeling program Hyperchem 7.0. The overall stabilization energy was calculated for each DNA-cisplatin complex using a thirteen base polynucleotide. We calculated the stabilization energy associated with cisplatin binding at four sites and compared these values to other binding sites. Relationships between the calculated binding energies and X-ray diffraction data of the cisplatin-DNA adduct were deduced. Using the cisplatin study as a model, we investigated the binding of six other inorganic complexes to the polynucleotide. These theoretical studies will be used as indicators of possible new inorganic drugs and DNA markers that have not yet been studied in the laboratory.

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SPECTROSCOPIC AND STRUCTURAL STUDIES OF A PALLADIUM(II) PYRROLATE-IMINE COMPLEX

The new complex Bis(2-*N*-benzyl-pyrrolylcarbaldimine) palladium(II) is isolated in good yield (~ 90%) from combination of the Schiff base 2-*N*-(benzyl)pyrrolecarbal dimine with a palladium(II) salt and base in methanol. The X-ray analysis shows *trans* geometry of the two pyrrolate-imine moieties around Pd(II) in a rigorously planar configuration; the bond lengths all lie within ranges expected for the atoms present, and the geometry found. With the exception of the imine benzyl substituents the remainder of the molecule can be considered as planar. The planes of the benzyl groups are canted at an angle of 83.6º above and below the coordination plane of the molecule, stacking to form parallel arrays throughout the crystal. Pyrrolate-imine coordination is inferred from infrared spectra by loss of n(N-H) and a shift (ca. 35 cm^{-1}) to lower energy for n(C=N) relative to free Schiff base. The ^{1}H-nmr spectra show that the C-H proton of the imine group is shifted about 0.70 d upfield in the complex relative to the ligand. The electronic absorption spectrum of the complex in chloroform shows only anticipated high-energy bands, which tail into the visible region to impart the orange color.

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SYNTHESIS OF TWO RIGID *m*-TERPHENYL DERIVATIVES WITH PERIPHERAL H-BONDING FUNCTIONAL GROUPS FOR USE AS TECTONS IN CRYSTAL ENGINEERING

Synthesis of two rigid *m*-terphenyl derivatives bearing *p*-substituted phenyl groups on C2' is described. The presence of peripherally placed H-bonding groups and the overall conformational rigidity of these molecules is expected to make these compounds useful building blocks (tectons) in crystal engineering. Key steps of the synthesis include a one-pot tandem aryne formation-nucleophilic capture reaction sequence and a subsequent Suzuki coupling reaction to introduce the C2' phenyl substituent.

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USING MOLECULAR MODELING TO PREDICT THE ULTRAVIOLET-VISIBLE SPECTRA OF C-40 HYDRO-CARBON CAROTENES

The prediction of the ultraviolet-visible spectra of C-40 hydrocarbon carotenes has been made by molecular modeling using the density functional B3LYP in the Spartan molecular modeling software. After geometric optimization the LUMO-HOMO transition correlates well with the published ultraviolet-visible spectral maxima and explains the spectral shifts seen in cis-trans isomers.

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THE USE OF RECYCLED SOYBEAN COOKING OILS IN MIDDLE DISTILLATE DIESEL FUELS

It has been suggested that renewable energy sources be considered as replacements or diluents for middle distillate ground transportation fuels. It is vital for the operational considerations of these fuels to investigate the many positives and negatives that this use could prompt. In proposing such a replacement, considerations must be given to the many problems that could arise. Problems to be studied include fuel storage stability, fuel solubility, and oxidative stability. Unlike newly manufactured soy oils, it was found that this recycled soy oil was not stable in fuels. The question was, what in the recycled oil leads to the observed fuel degradation.

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