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15. Pharmacy

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05. Mathematics and Science

15. Pharmacy

05.15.01 Evaluation of the Physicochemical Properties of a Novel Antimalarial Drug Lead, Cyclen Bisquinoline

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The purpose of this study was to evaluate physicochemical properties of a novel antimalarial drug lead, 4,10-bis (7-chloroquinoline)-1,4,7,10-tetraazacyclododecane (free base; FB) and its hydrochloride salt. Differential scanning calorimeter (DSC) was employed to determine and quantify the energy of phase transition and conformational changes. Equilibrium solubility and stability of both FB and its salt were carried out in different mediums, and samples were analyzed using RP-HPLC. pKa values were calculated by both pH-metric and UV-metric methods. The log P value of the compound was determined by RP-HPLC from the best fit calibration curve of log P vs. log k values of the reference standards. The FB is a white polymorphic crystalline powder; the polymorphs melt at 166, 178, 195, and 234°C, respectively. The salt is off-white powder that showed a broad endotherm in DSC analysis suggesting it to be amorphous. Both forms were stable in a wide range of conditions (acid, base, water, light and heat) except oxidation. Three pKa values, 5.9, 6.6 and 8.7, were obtained for the compound. It has a log P value of 5.14. The application of standard experimental protocol revealed that the compound has at least four different crystalline polymorphs. It is highly hydrophobic; however, salt formation improved its water solubility by approx. 370-fold. All these properties would be useful in implementing the modern quality by design approaches for further development of the drug lead.
05.15.02  **UV-Metric, pH-Metric and RP-HPLC Methods to Evaluate the Multiple pKa Values of a Polyprotic Basic Novel Antimalarial Drug Lead, Cyclen Bisquinoline**

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The purpose of this experiment was to evaluate and compare the pKa values of the poorly water soluble, weakly basic, novel antimalarial drug lead, 4,10-bis (7-chloroquinoline)-1,4,7,10-tetraazacyclododecane (CNBQ). Three separate methods, pH-metric, UV-metric, and reverse phase-high performance liquid chromatography (RP-HPLC), were employed to determine the pKa values between 2.0-12.0 pH range. The acetate and phosphate buffers, in addition to methanol and acetonitrile as co-solvents and potassium chloride to maintain the ionic strength, were used as appropriate. In UV-metric method, the drug substance is dissolved in aqueous media eliminating any interference of a co-solvent for measuring the pKa. Consequently, the pKa values obtained by the UV-metric method are considered accurate, as opposed to potentiometric and RP-HPLC methods that require the use of co-solvents. Thus, through the utilization of UV-metric method three pKa values, 5.9, 6.6, and 8.7, were obtained for CNBQ. These studies would be useful to determine the pKa values of the related drug leads under development.

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05.15.03  **Healthy Mouth, Healthy Heart**

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Lauren, Martinez Scobell  *Northwestern Oklahoma State University*

Lori, Shearer  *Northwestern State University*

Do patients that receive prophylactic antibiotics before a dental procedure have a decreased risk of developing infective endocarditis compared to patients that do not receive prophylactic antibiotics before a dental procedure? The prophylactic use of antibiotics has been highly recommended for dental procedures for many years. Since the American Heart Association updated their guidelines, the use of antibiotics prior to a dental procedure has greatly declined. Currently, it is recommended that patients only receive these antibiotics if they have a history of heart disease, congenital heart defects, heart transplant, past diagnosis of infective endocarditis, prosthetic valve or valve repair. The American Heart Association is changing the focus from prophylactic use of antibiotics to improved oral health overall. Antibiotics often have some negative side effects related to them as well as our bodies built immunity to these medications. The treatment regimen is often not followed as it should be, therefore, they are not as effective. The over use of antibiotic can decrease the effectiveness of the medication when it is needed for an infection. This research aims to show the use of prophylactic antibiotics prior to dental procedures is not always a necessity.
Towards the Synthesis of N4O2-Type Metal Complexes of Antimalarial Macrocyclic Polyamine Ligands

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The purpose of this study is to synthesize a series of N4O2-type stable metal complexes of antimalarial macrocyclic polyamine drug leads. The synthetic strategy relies upon the well-defined regioselective synthesis of tetracyclic derivatives of cyclen and related polyamines. First step of the method started with the synthesis of cyclen glyoxal followed by the synthesis of 1,7-dibenzyl-cyclen glyoxal 1,7-bisquaternary ammonium salt. Hydrolyzing the salt leads to the formation of 1,7-dibenzyl-cyclen proceeded by the synthesis of 4,10-bismethylacetyl 1,7-dibenzyl cyclen. Hydrogenolysis was performed on this product to yield 1,7-bismethylacetyl cyclen. This product was further treated with 4,7 dicycloquinoline to obtain the 1,7-bismethylacyl l-4,10-bis (dicloquinoline) cyclen. The N4O2-type metal complexes of the ligand will be synthesized by hydrolyzing this ester product to carboxylate, and then reacting with metals.