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Exploring the antituberculosis potential of Schiff-base transition metal complexes: Synthesis and characterization of copper (II) and cobalt (II) complexes of 5-(substituted-salicylidene) amino pyridine

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Treatment of tuberculosis (TB) still remains an important and challenging problem because of a combination of factors including increasing the number of multi-drug resistance to the existing tuberculosis drugs and comorbidity of TB with HIV. The World Health Organization recently reported TB as one of the leading cause of death from infectious disease especially in Africa. Discovery of new compounds with anti-tuberculosis (anti-TB) effect and possibly with mechanism of action different from those of well-known TB drugs is highly desirable. Schiff-bases and their metal complexes represent major investigational compounds. The Schiff-bases were obtained by the condensation reaction of salicylaldehyde with 2 (L1-L4) and 4-aminopyridine (L4-L7). They were reacted with $CuCl_2.H_2O$ and $CoCl_2.6H_2O$ to form Cu (II) and Co (II) complexes. ^1H, ^{13}C NMR, IR, electronic absorption and elemental analysis confirm the formation of the ligands. The metal complexes were also characterized on the basis of various spectroscopic techniques. The compounds were screened for their anti-TB activity using the proportion method and isoniazid (INH) as a reference compound. The complexes showed enhanced *in-vitro* anti-tuberculosis activity against *Mycobacterium tuberculosis* $H_{37}RV$ compared to the free ligands and the reference compound (INH). Co (II) complex containing the nitro substituent exhibited significant anti-TB activity with an MIC of 0.05 µg/mL, the results demonstrate that compounds with imine group and metal ion can display strong anti-TB activity making them suitable as lead compound in the development of new TB drugs.

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Optimization of rate of chemical reaction using nature inspired optimization algorithms

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Chemical reaction involves transformation of reactant into product. Rate of chemical reaction is the measure of how fast these changes are taking place. Some reactions occur very rapidly, others very slowly. For example, ionic reactions are very fast, while those taking place in water treatment plant may last upto few days. The speed at which the reaction happens is the rate of chemical reaction. If a chemical reaction has high rate, shows that molecule combines at a higher rate than the reaction has slow rate. The rate of chemical reaction can also depend up on the type of molecules that are combining. If there are low concentration of an essential element or a compound, the reaction will be slower. In this paper we present optimized rate of chemical reaction using for different nature inspired algorithms i.e. random, Genetic Algorithm, Differential Evolution and Particle Swarm Optimization to maximize the rate of chemical reaction. Tests show that different algorithms perform significantly better for different reactions and have different convergence rate. In this paper, we use an object-oriented software tool named Cantera to calculate the rate of reaction which uses modified Arrhenius equation. Cantera is a software tool to solve the problems in the fields of transport processes, chemical kinetics and thermodynamics: Problems related to combustion, electrochemical energy conversion, storage and rate of chemical reaction can be solved using Cantera. We can use Cantera from Forton 90 or C++ based application. In this paper we have used python interface because there are many advantages for choosing python over any other language as it covers almost all the features of basic C++ and object-oriented concepts and in addition it provides a flexible environment. Cantera uses modified Arrhenius equation for getting value of rate constant r=PK^n.e^(-Ea/GK).

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