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Synthesis and biological evaluation of Schiff base derivatives of furfural based heterocyclic flavonoids

Hari Babu Bollikolla and **Bala Murali Krishna Khandapu**
Acharya Nagarjuna University, India

Synthesized a total number of 12 new furfural flavone Schiff base derivatives starting from commercially available phloroglucinol. In the first stage of the corresponding acetophenone key intermediate was synthesized from the starting material and was condensed with furfural followed by cyclisation, and formylation. Finally, the formylated flavone was condensed with various aromatic primary amines to obtain the desired Schiff base derivatives. All the synthesized furfural flavone Schiff base derivatives were tested for their anticancer and antibacterial activities and the results were analysed in the light of their structural activity.

dr.b.haribabu@gmail.com

Optimization of rate of chemical reaction using nature inspired optimization algorithms

Harnoor Singh Kaler
Thapar Institute of Engineering and Technology, India

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 up to 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 on type of molecules that are combining. If there is low concentration of an essential element or 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. About Cantera: 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).

hskaler98@gmail.com

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