Abstract

Title : "*Sterculia foetida* - Eco-friendly, cost effective and rich sources of nutritious edible oil, animal food supplements as well as biofuel and to evaluate its antimicrobial and cytotoxic efficacy by comparing with other edible vegetable oils to validate its pharmaceutical application".

Submitted by- **Rahul Bose**
Index No.- **56/18/Life Sc./25**

Medicinal plants have long been used in the prevention and cure of various diseases of the humans and the animals. *Sterculia foetida* seed oil consists of the two unusual fatty acids namely sterculic acid, malvalic acids with cyclopropane functionality. Seeds of *Sterculia foetida*, L. yielded considerable amount of oil (58.7g/100g) as compared to other edible vegetable oils (such as sunflower, ground nut, mustard, soybean). Fatty acids composition of all the five tested oils showed that total fatty acid as well as unsaturated fatty acid percentage is higher in Sterculia seed oil. Proximate and mineral composition analysis suggested that Sterculia oil is a good source of protein, lipids, macro and micronutrients. Lowest TOTOX value (2.67) and higher iodine value (132-144) indicated its higher oxidative stability and presence of greater number of unsaturated bonds in the fatty acid moieties which is also beneficial for human health. Sterculia oil exhibited lower IC_{50} values in DPPH (825.73 µg/ml), ABTS (225.23 µg/ml) and NO (111.98 µg/ml) radical scavenging assays, only sunflower and mustard oils showed significant differences in IC_{50} values in DPPH assay. Sterculia oil did not exhibit any cytotoxic effect on both normal and cancerous cell lines even at concentrations of 40µg/ml as evident from MTT assay.Antimicrobial, cytotoxic and molecular docking study (with Bax and MDM2) of bromosterculic acid [8-(1, 2-dibromo-2-octylcyclopropyl)octanoic acid], a new synthetic derivative of *Sterculia foetida* seed oil was assessed to validate its pharmaceutical potentiality. Bromo-sterculic acid was prepared by bromination of sterculic acid and its structure was confirmed by Mass spectrometry.This synthetic derivative showed strong fungicidal activity against two pathogenic fungal species namely *Penicillium chrysogenum* and *Aspergillus niger* with minimum inhibitory concentration (MIC) of 0.007 mg/mL and strong bactericidal activity against *Bacillus subtilis* and *Xanthomonas* sp.with MIC of 0.015 mg/mL. Cytotoxic activity on both normal (MCF-10A) and cancerous (MDA-MB-468) cell lines revealed that survivability rate of normal cells were unaffected, whereas cancerous cells were decreased greatly by bromo-sterculic acid at doses less than 5µg/mL. Molecular docking using AutoDock 4.2 showed that bromosterculic acid binds to Bax with the best conformation that has a minimum free binding energy of -11.4kcal/mole. It makes strong pi-sigma interaction with PHE-93, pi-alkyl and alkyl interaction with TRP-139, ARG-89 and PHE-92. The best conformation of bromosterculic acid that binds to MDM2 has −11.6 kcal/mol binding energy. It makes strong hydrogen bond interaction with GLN-59 and pi-alkyl interaction with PHE-55.

Suparna Mandal Biswas

Signature of the supervisor

Dr. Suparna Mandal Biswas
Associate Professor
Agric. & Ecol. Res. Unit
Indian Statistical Institute
203, B.T. Road, Kolkata-700 108, India

Rahul Bose 06.07.22

Signature of the candidate