

## Optimization of process parameters of hydraulic press for coconut oil yield using RSM and artificial neural networks

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Most oilseeds (eg copra, palm kernels and groundnuts) need proper processing in mills before oil extraction to increase the yield of oil. The efficient and economical utilization of feed stocks is highly essential in oil producing industries. Coconut has the highest productivity and is less susceptible to abnormal climatic condition. The production of coconut oil and its by-products, raw and fried cake, is an important source of income for women in coastal areas of India. Hence, identification of optimal pretreatment conditions of coconut nut kernel is very important for high yield of coconut oil. The optimum processing conditions can be found by incorporating reliable and efficient statistical design methodologies such as central composite design (CCD), and ANN.

Response Surface Methodology was used to conduct the experiments and experiments were designed according to CCD to study the effects of process variables such as Applied pressure, Pressing time, Roasting temperature, Roasting time and Moisture content. A simple, economical, and highly efficient model was developed to predict the yield of oil from coconut kernels in a hydraulic press. Artificial neural network (ANN) model was developed to predict the yield of oil from coconut kernels. The developed ANN was trained and tested with the experimental data obtained from CCD method. The results of ANN during training and testing were based on MSE. The results were compared with experimental data and it was found that the estimated oil yield from ANN model was able to predict the yield accurately with R value as 0.99.

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## Novel acridinedione derivatives: Design, synthesis, SIRT1 enzyme and tumor cell growth inhibition studies

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A new scaffold N-(9-(ortho/meta/para -(benzyloxy)phenyl)-3,3,6,6-tetramethyl-1,8-dioxo-1,2,3,4,5,6,7,8-octahydroacridin-10(9H)-yl) isonicotinamide (H1-3) was discovered as a hSIRT1 inhibitor through virtual screening of in-house database. Based on these hits, a library of compounds were designed, synthesized and tested for in-vitro hSIRT1 activity. The most potent compound 4d in the series showed a significant inhibition of SIRT1 activity. Further antitumor studies of compound 4d, showed a dose dependent increase in acetylation of p53K382 and decrease in SIRT1 with an IC<sub>50</sub> of 0.25 μM in MDA-MB231 breast cancer cell lines. Individual 3D- QSAR analysis using Schrödinger showed distribution of hydrophobic and non-polar positive co-efficient at ortho position essential for bioactivity based on 4d.

**Keywords:** Antiproliferative activity, Acridinedione derivatives, hSIRT1, MDA-MB231.

### Biography

Alvala Mallika pursuing her Ph.D from Birla Institute of Technology and Sciences, Pilani, Hyderabad Campus and completed her Master's Degree in Pharmacy from Birla Institute of Technology and Sciences, Pilani, India. She has published 8 papers in reputed journals and serving as a reviewer for the reputed journal 'Pharmaceutical Biology'. Her research areas include designing of small molecule modulators against various targets in cancer, Obesity and TB based on molecular mechanisms using computational approach, cell based assays and in vitro screening of validated targets.

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