Estimation of total alkaloids in Cinchona bark using a developed portable NIR

Presenter:
Rajib Bandyopadhyay
Dept of Instrumentation and Electronics Engg
Jadavpur University
E-mail: bandyopadhyay.rajib@gmail.com
rajib.bandyopadhyay@jadavpuruniversity.in
Cinchona Tree
Global Quinine Market Review

- The global demand for quinine market was valued at approx. **USD 804.98 M** in **2018**
- Predicted revenue around **USD 1,184.15 M** by end of **2025**
- **CAGR** of around **5.68%** between **2019** and **2025**.

PR Newswire on Jan 03, 2020
Application of the Quinine

- Problematic leg cramps
  - Malaria
  - Quinine sulphate is commonly used to treat painful leg cramps.

Malaria
- Nearly half the world’s population lives in areas at risk of malaria transmission in 87 countries and territories, reported by CDCP, December 16, 2021
- The estimated number of malaria deaths stood at 627,000 in 2020, as per the WHO.

Leg cramps
- Nocturnal leg cramps affect about 6% of the American population, whose condition seems related to heart problems and depression, NCBI

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INPORTANT FORMULATION OF QUININE:
Tonic water is a soft drink containing quinine, which gives it a bitter taste. Quinine is a common treatment for malaria. Some people believe that it can also help with leg cramps and restless legs syndrome. Quinine comes from the bark of the cinchona tree.

Global Tonic Water Market
OPPORTUNITIES AND FORECAST, 2021-2027

Global Tonic Water Market is expected to reach $1.1 Billion by 2027.
Growing at a CAGR of 7.3% (2021-2027)

The key players operating in the Quinine market:
Aecochem Corp  Haihang Industry Co. Ltd.
Actavis  Shreeji Pharma International
Wockhardt  B. Enterprises
Hangzhou Dayang Co. Ltd.IS Chemical Technology Ltd.
Trademax Pharmaceuticals & Chemicals
Caraco Pharmaceutical Laboratories
OBJECTIVES

The Government of WB, India, Cinchona Plantation comprise at the Rangju Valley block, consisting of the Rangbi and Mungpoo Divisions, which together measure about 900 acres, containing nearly over 2 million plants.

Currently, available analytical methods are based on wet chemistry procedures without data-driven or AI-based approaches such as
- High-pressure liquid chromatography,
- Thin-layer chromatography, and
- Microscopic analyses,
- Time consuming process, very lengthy
- Sample destruction
- Complex
- High cost
- Professional skill is required and lab based
NIR spectrometer

Block diagram of optical assembly of NIR spectrometer
NIR Spectrometer

Optical Assembly of NIR spectrometer
The portable NIR Spectrometer

- The Latte Panda Delta 432 with a 7” touch display panel used in place of the laptop/computer.
- The complete setup is housed in an enclosure.
**Data Capture with plot of Tab Wavelength (in nm) versus absorbance**

**Real-time prediction of concentration of bio-marker in plant**
Absorbance vs wavelength plot for Cinchona

<table>
<thead>
<tr>
<th>Spectra / plot</th>
<th>Peak</th>
<th>Corresponding Chemical Bond</th>
</tr>
</thead>
<tbody>
<tr>
<td>Raw</td>
<td>1450 nm</td>
<td>N-H and OH 1st overtone</td>
</tr>
<tr>
<td></td>
<td>905 nm, 915 nm, 925 nm, 930 nm</td>
<td>C-H 3rd overtone</td>
</tr>
<tr>
<td></td>
<td>955 nm</td>
<td>O-H 3rd overtone</td>
</tr>
<tr>
<td></td>
<td>1430 nm</td>
<td>C-H 2nd overtone</td>
</tr>
</tbody>
</table>
## Results and Discussion

Quinine concentration in the measured Cinchona samples used for calibration and prediction sets.

<table>
<thead>
<tr>
<th>Sample Sets</th>
<th>No. of Samples</th>
<th>Min(mg/g)</th>
<th>Max(mg/g)</th>
<th>Mean(mg/g)</th>
<th>Median(mg/g)</th>
<th>Standard Deviation(mg/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Samples</td>
<td>30</td>
<td>1</td>
<td>8.07</td>
<td>3.194</td>
<td>2.58</td>
<td>1.708</td>
</tr>
<tr>
<td>Calibration Set</td>
<td>25</td>
<td>1</td>
<td>8.07</td>
<td>3.113</td>
<td>2.57</td>
<td>1.632</td>
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<tr>
<td>Prediction Set</td>
<td>5</td>
<td>1.3</td>
<td>8.07</td>
<td>3.519</td>
<td>2.97</td>
<td>1.986</td>
</tr>
</tbody>
</table>
Performance of PLSR full-band models using developed NIR spectrometer for predicting quinine concentration in Cinchona

<table>
<thead>
<tr>
<th>Model</th>
<th>Parameters</th>
<th>Calibration</th>
<th>Prediction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LV</td>
<td>$R_c^2$</td>
<td>$R_p^2$</td>
</tr>
<tr>
<td>PLS</td>
<td>10</td>
<td>0.98</td>
<td>0.20</td>
</tr>
</tbody>
</table>
Results and Discussion

Calibration plot by PLSR for cinchona

Prediction plot by PLSR for cinchona
## Results and Discussion

### Estimated concentration of Quinine in five unknown Cinchona samples

<table>
<thead>
<tr>
<th>Actual concentration of Quinine in Cinchona (Gravimetric method)</th>
<th>Predicted concentration of Quinine in Cinchona (Developed NIR)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.31</td>
<td>2.62</td>
</tr>
<tr>
<td>2.41</td>
<td>2.59</td>
</tr>
<tr>
<td>2.53</td>
<td>2.53</td>
</tr>
<tr>
<td>3.88</td>
<td>3.75</td>
</tr>
<tr>
<td>7.6</td>
<td>7.42</td>
</tr>
</tbody>
</table>
Conclusion and Future scopes

➢ Conclusion
  • Design and development of a portable NIR spectrometer with GUI.
  • Quinine content estimated by NIR spectrometer
  • It fulfills the requirements according to AACC Method 39-00 (AACC Method, 39-00:15, 1999) to be used at least for screening (RPD ≥2.5).

➢ Future scopes
  • More number of samples would be used for model development.
  • Integration of IoT to store the data in cloud and access by mobile at any time and anywhere.
  • Use of Blockchain for security and transparency throughout the value chain.
Thank You