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

Presenter:

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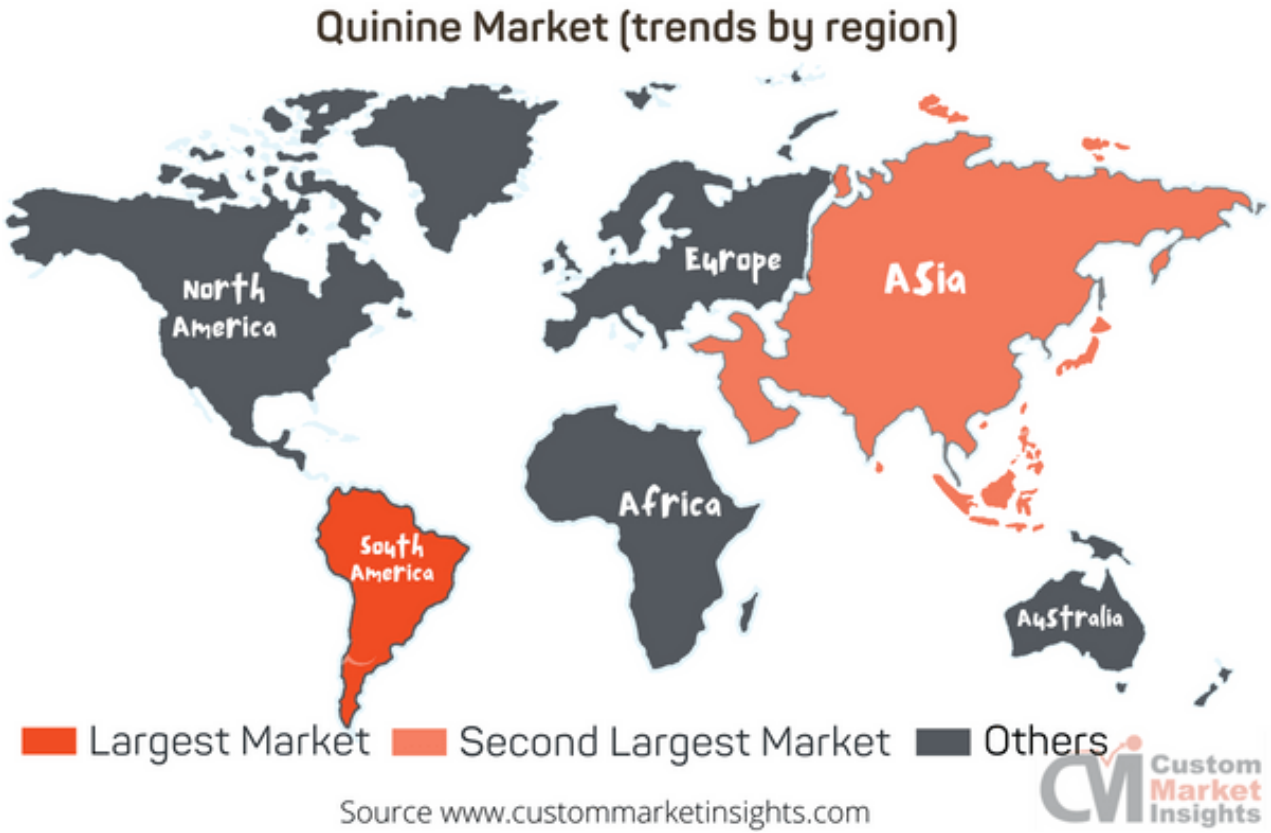
Cinchona Tree

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

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.

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

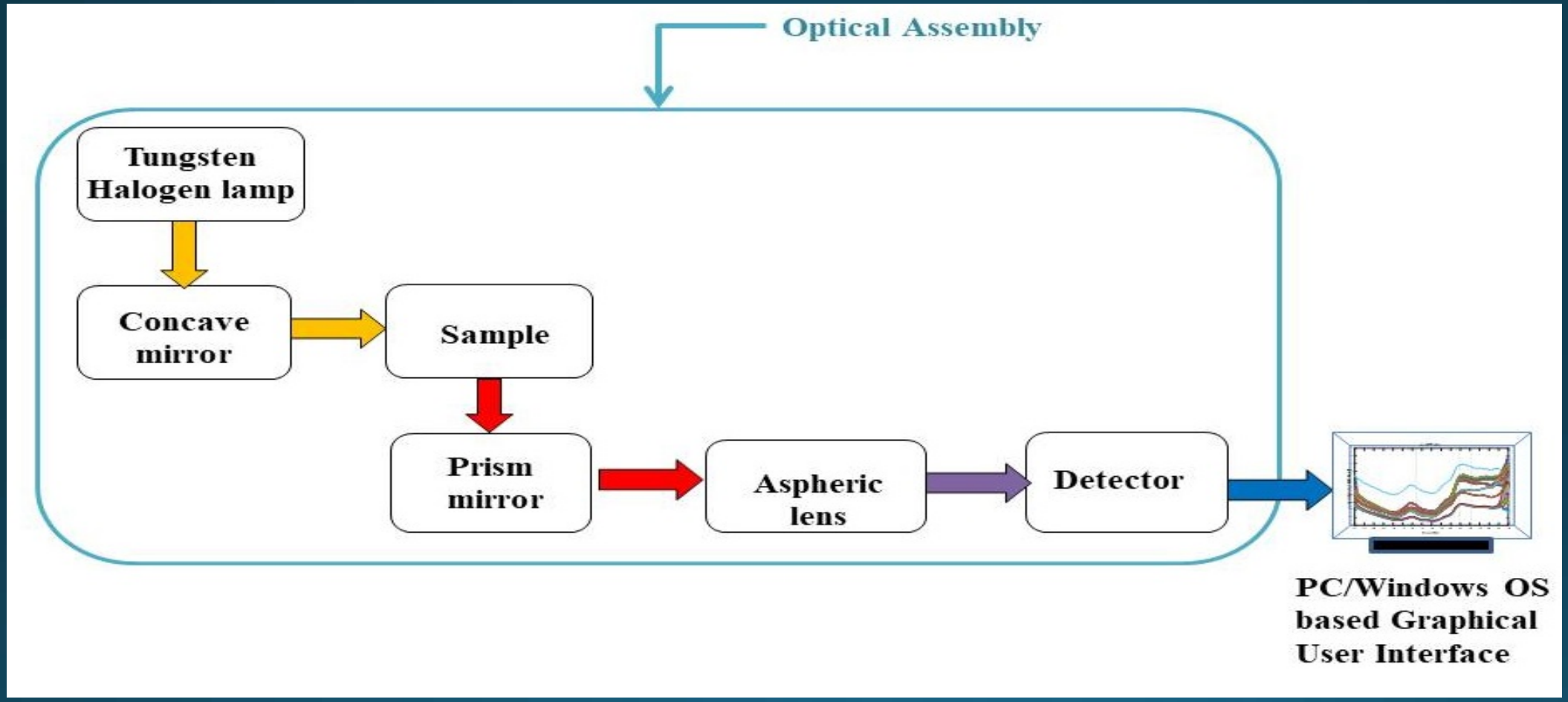
OBJECTIVES

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

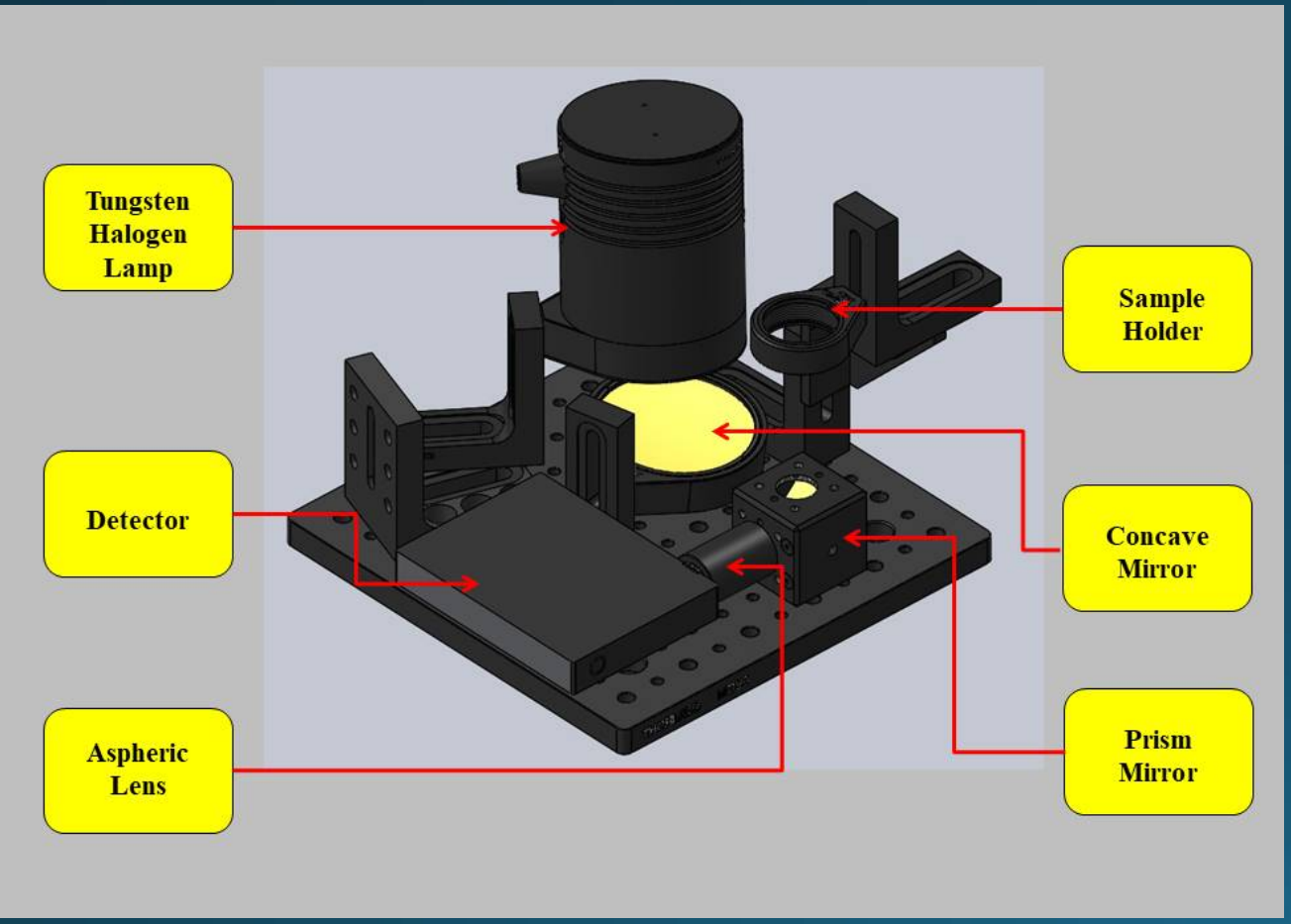
NIR spectrometer

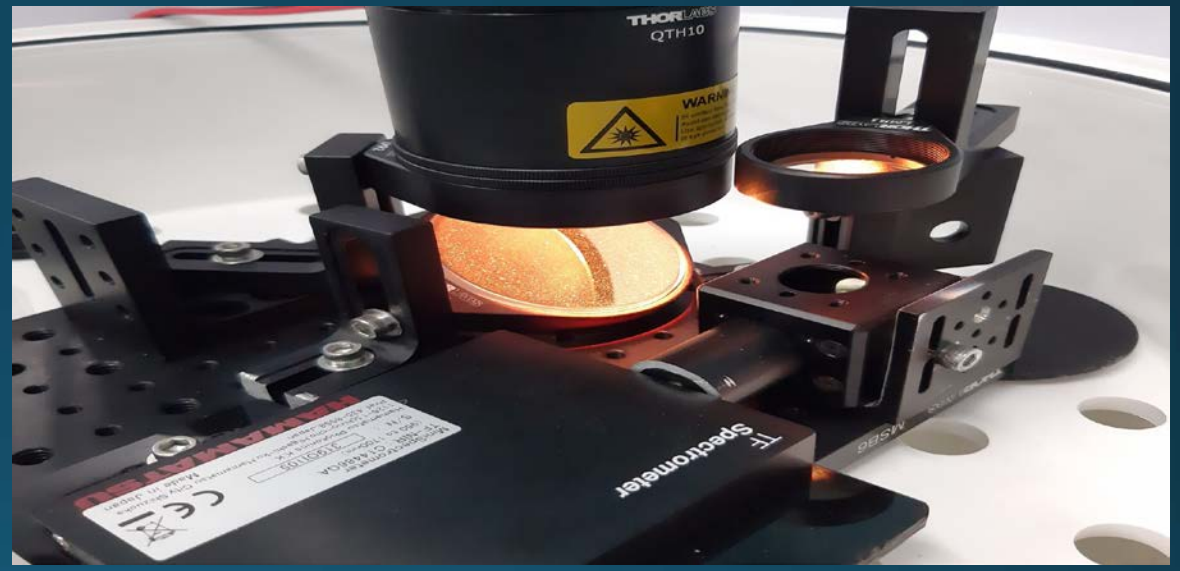


Block diagram of optical assembly of NIR spectrometer

NIR Spectrometer

Optical Assembly of NIR spectrometer





The portable NIR Spectrometer

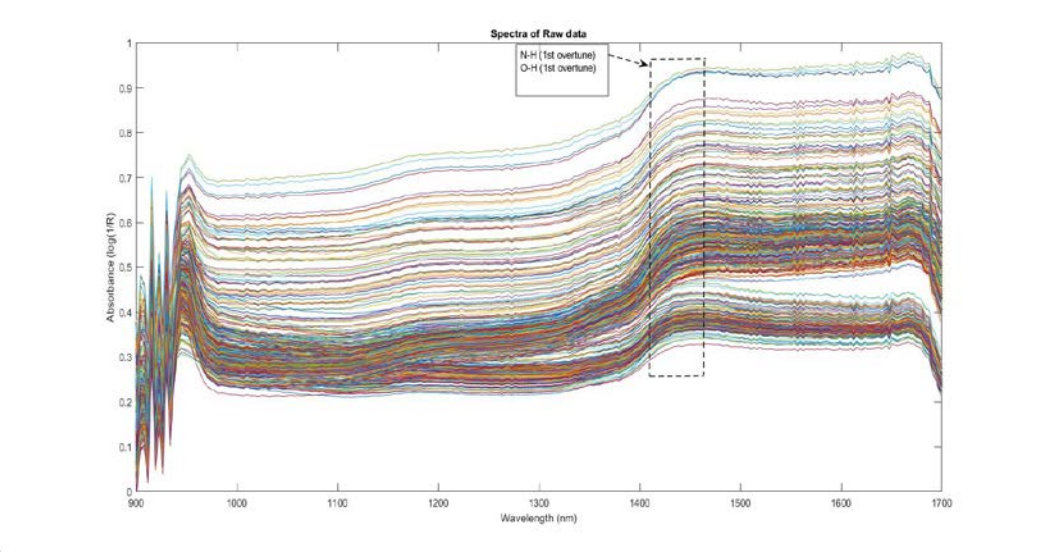
- The Latte Panda Delta 432 with a 7” touch display panel used in place of the laptop/computer.
- The complete setup is housed in an enclosure.

GUI of developed portable NIR spectrometer

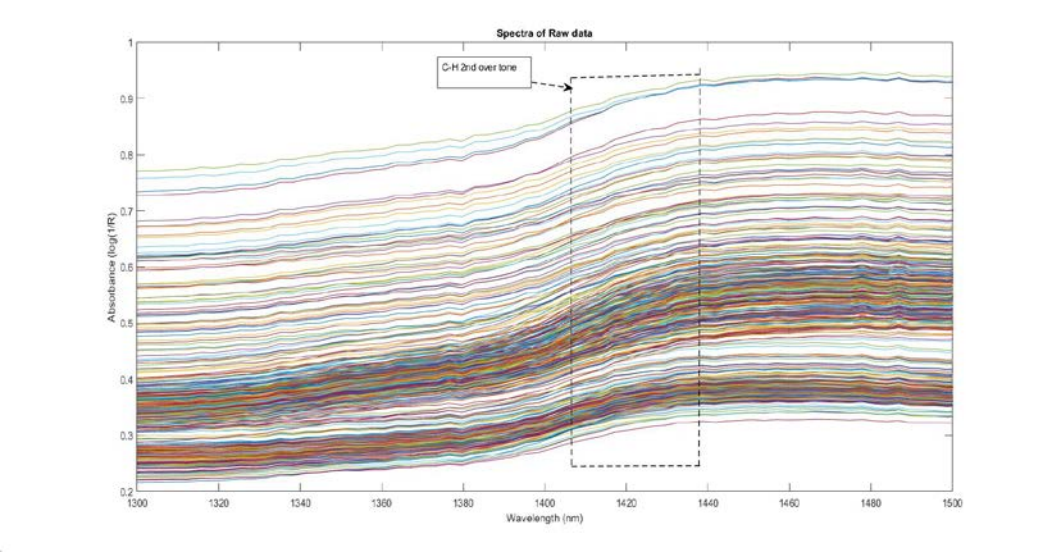
Data Capture with plot of Tab Wavelength(in nm) versus absorbance

Real-time prediction of concentration of bio-marker in plant

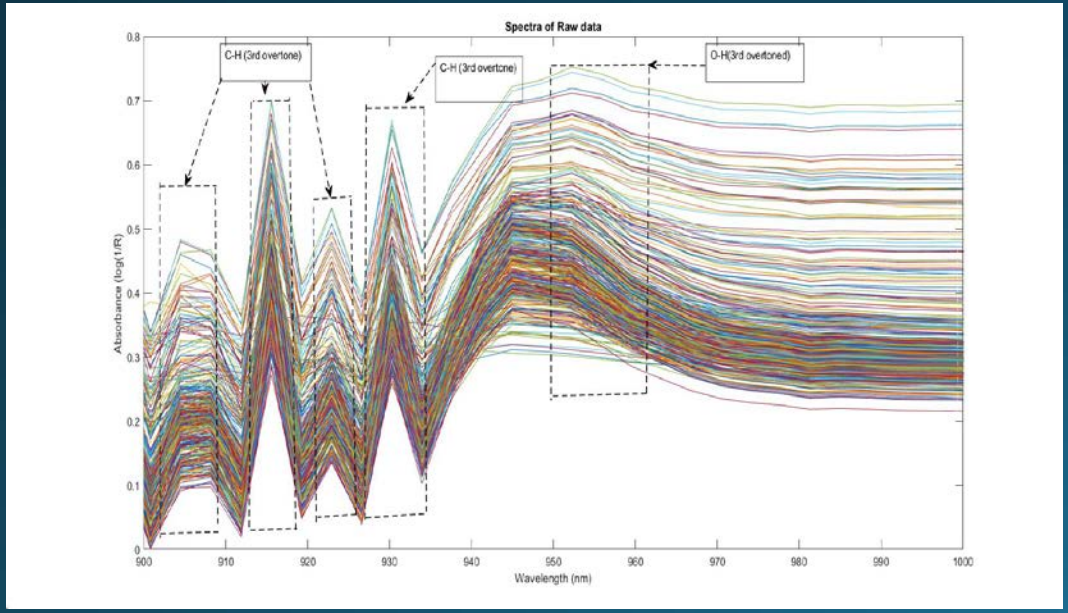
Absorbance vs wavelength plot for Cinchona



Overall 900nm to 1700nm



Zoomed version 1300nm to 1500nm



Zoomed version 900 nm to 1000 nm

Spectra / plot	Peak	Corresponding Chemical Bond
Raw	1450 nm	N-H and OH 1st overtone
	905 nm,915 nm,925nm,930nm	C-H 3rd overtone
	955 nm	O-H 3rd overtone
	1430 nm	C-H 2nd overtone

Results and Discussion

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

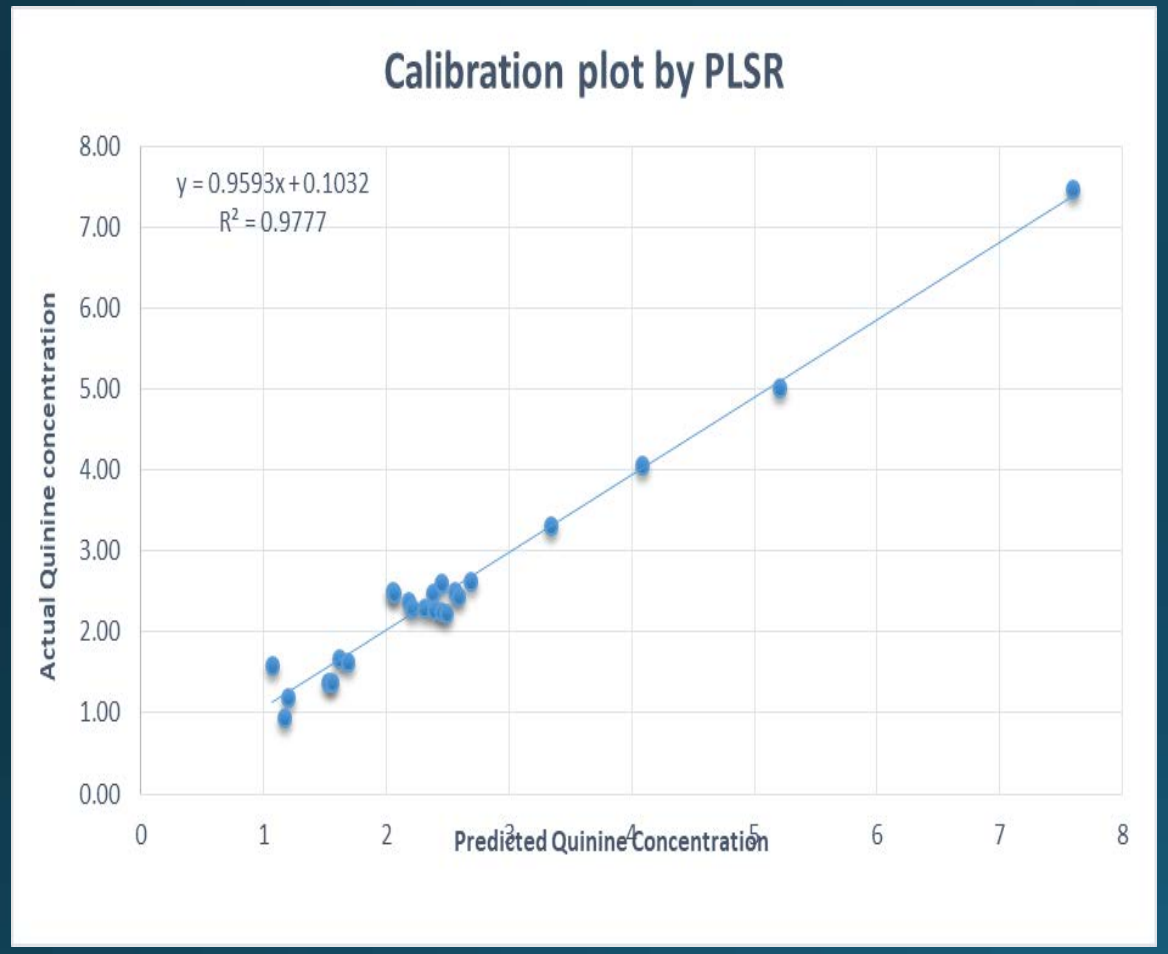
Sample Sets	No. of Samples	Min(mg/g)	Max(mg/g)	Mean(mg/g)	Median(mg/g)	Standard Deviation(mg/g)
Total Samples	30	1	8.07	3.194	2.58	1.708
Calibration Set	25	1	8.07	3.113	2.57	1.632
Prediction Set	5	1.3	8.07	3.519	2.97	1.986

Results and Discussion

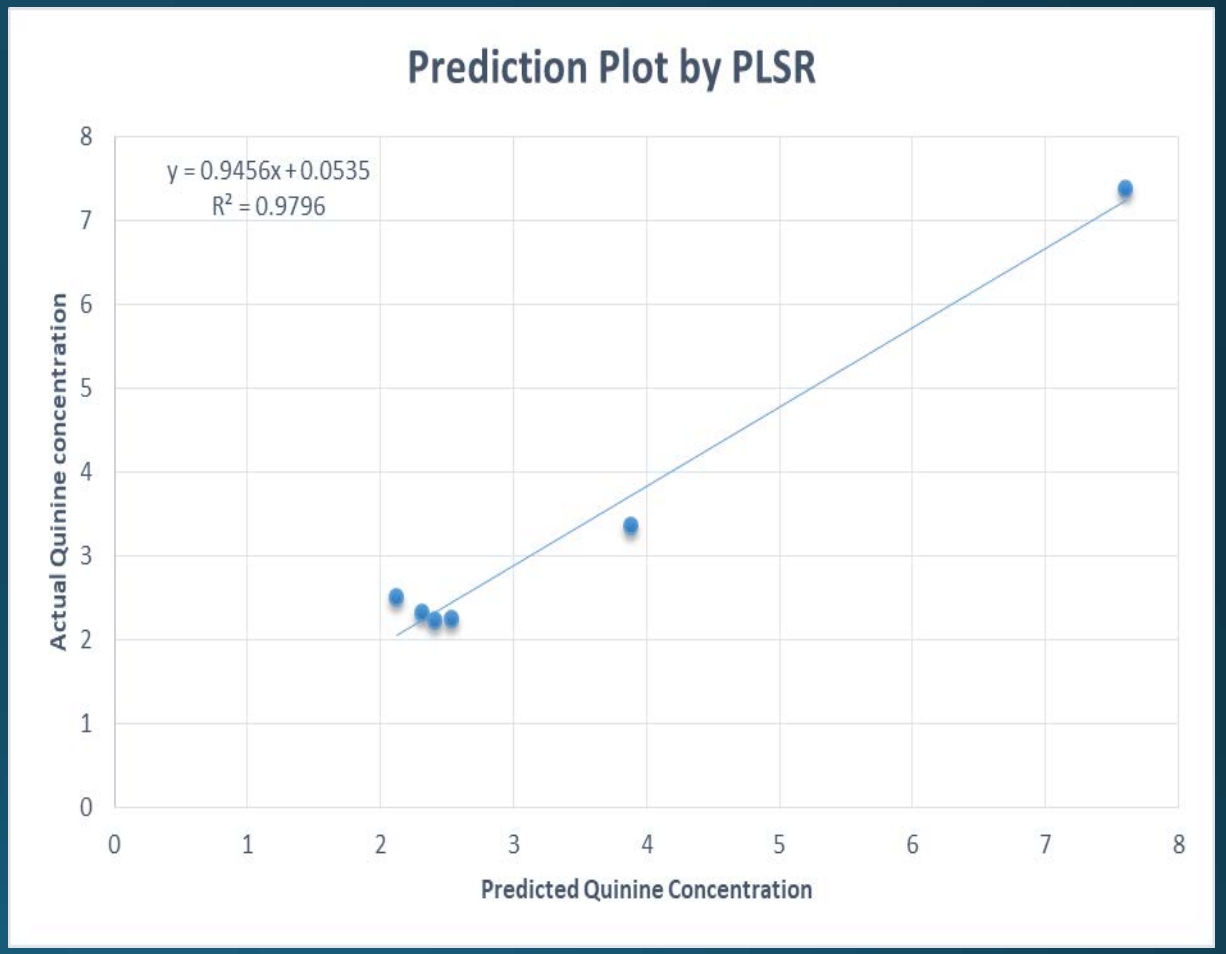
Performance of PLSR full-band models using developed NIR spectrometer for predicting Quinine concentration in Cinchona.

Model	Parameters	Calibration			Prediction		
PLS	LV	R_C^2	$RMSE_C$	RPD_C	R_P^2	$RMSE_P$	RPD_P
	10	0.98	0.20	6.64	0.98	0.32	6.13

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

Actual concentration of Quinine in Cinchona	Predicted concentration of Quinine in Cinchona
(Gravimetric method)	(Developed NIR)
2.31	2.62
2.41	2.59
2.53	2.53
3.88	3.75
7.6	7.42

Conclusion and Future scopes

- Conclusion
- Design and development of a portable NIR spectrometer with GUI.
- Quinine content estimated by NIR spectrometer
- It fulfils 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 through out the value chain.

Thank You