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Data Article

Rheological and NMR spectral data sets of quaternary ammonium derivative of *Cassia tora* Linn. seed gum

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ABSTRACT

The present study has been carried out to investigate the rheological and spectral data of galactomannan and its quaternary ammonium derivative obtained from the endosperm of *Cassia tora* Linn. seed. The characterization of native and quaternized *Cassia tora* gum (CTG) was done by employing 2D NMR spectroscopy including HSQC and HMBC spectra. The data was analysed to identify the quaternary ammonium moiety introduced onto the galactomannan chain. The correlation signal of carbon and hydrogen of quaternary ammonium groups introduced onto the galactomannan chain was observed at 56 and 2.7 ppm respectively in HSQC spectrum. Further, the rheological data of CTG and derivatized product has been discussed. The data is related to the research article *"Synthesis and characterization of quaternized Cassia tora gum using Taguchi's L′16 approach"* [1].

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Specifications Table

Subject	Chemistry
Specific subject area	Rheological and 2D NMR spectral datasets for structural characterisation
Type of data	Figure and table
How data were acquired	NMR: Bruker Advance Neo 500 MHz NMR spectrometer Rheological data: Brookfield DV-III Ultra digital Viscometer
Data format	Raw data analysed and graph a) NMR analysis of native and quaternized CTG b) Rheological data of native and quaternized gum
Parameters for data collection	The NMR spectra was recorded using following parameters: Solvent: D_2O Temperature (K): 303.3 Spectrometer frequency (MHz): 500.17 (^1H) & 125.77 (^{13}C) Number of scans: 2 (HSQC) & 8 (HMBC) Relaxation delay(sec): 1.5 Acquisition time (sec): 0.1946 Spectral width (Hz): 1315.8, 27672.1
Description of data collection	The gum (CTG) was obtained from the endosperm of *Cassia tora* seeds. Quaternisation of CTG was done by employing different reaction parameters. NMR spectral data of the native and quaternized CTG were recorded and data sets were interpreted. Rheological data was also collected.
Data source location	Institution: Forest Research Institute, Dehradun & Sophisticated Analytical Instrument Facility (SAIF) Chandigarh City: Dehradun, Chandigarh Country: India
Data accessibility	The raw data files are provided as the supplementary files. All other data is with this article.
Related research article	The data is related to the research article: Authors: Deepak Sharma, Vineet Kumar, Raman Nautiyal & Pradeep Sharma Title: 'Synthesis and characterization of quaternized Cassia tora gum using Taguchi's L'16 approach' Journal: Carbohydrate Polymers [1] DOI/In Press: https://doi.org/10.1016/j.carbpol.2019.115731

Value of Data

- The spectral data set values are significant for interpretation and structure elucidation of native and quaternized *Cassia tora* gum.
- HSQC and HMBC NMR spectral data of samples viz. native and quaternized *Cassia tora* gum were recorded in order to characterize and build up systematic data sets. The study will be helpful to the researchers for correlation studies (proton and carbon) of native and derivatized gum using HSQC and HMBC NMR spectra.
- Rheological data sets of samples viz. native and modified gum were studied to investigate the viscosity and stability of the derivatized samples. The rheological data will be helpful to scientific community to provide an insight for industrial aspects of derivatized gum for end-use applications.
- The study would provide a lead to researchers for future scientific investigation of structural and rheological aspects of native and quaternized polysaccharides in general and galactomannans in particular.
- The data also provides different steps involved in isolation of *Cassia tora* gum powder from leguminous plant.

1. Data description

The data which has been presented here include the following points:

- Fig. 1 illustrates different stages to obtain *Cassia tora* gum from legumes and derivatisation of gum sequentially viz. a) wildly available *Cassia tora* legumes from plant b) seeds obtained from legumes c) endosperm from the seeds d) *Cassia tora* gum e) quaternized derivative of *Cassia tora* gum.
- Figs. 2 and 3 illustrate the HSQC spectra of native and quaternized *Cassia tora* gum, Figs. 4 and 5 illustrate the HMBC spectra of native and modified *Cassia tora* gum. Raw experimental records

Fig. 1. Optical images of (a) legumes from *Cassia tora* plant (b) seeds of *Cassia tora* (c) endosperm of *Cassia tora* (d) *Cassia tora* gum (e) quaternized *Cassia tora* gum.

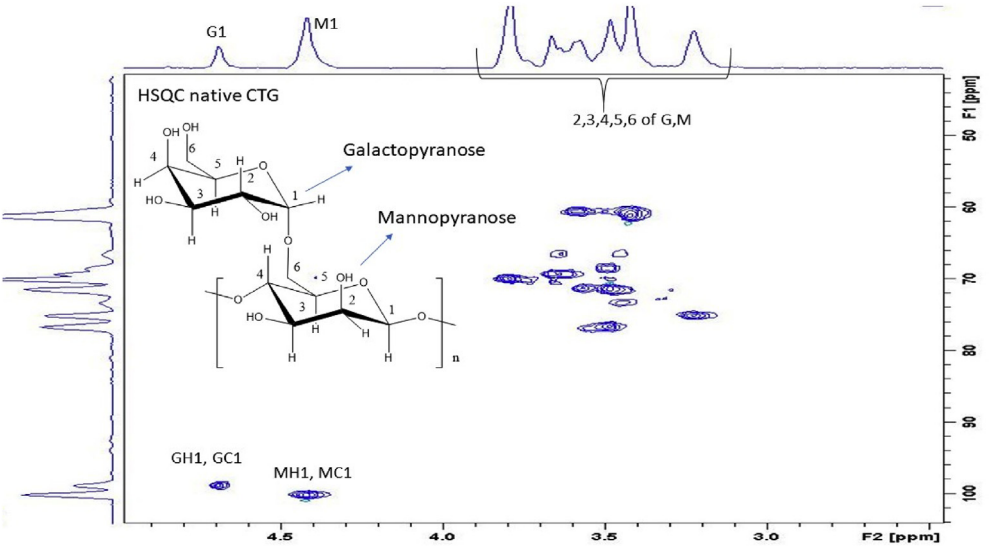

Fig. 2. HSQC spectra of *Cassia tora* gum.

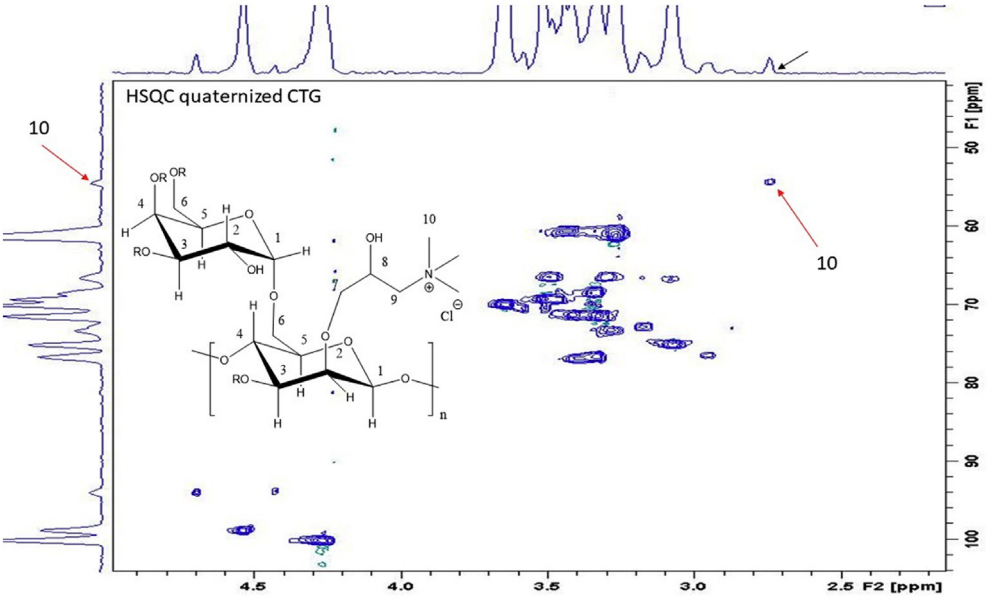

Fig. 3. HSQC spectra of quaternized *Cassia tora* gum.

are extremely large. The obtained raw data from NMR instrument was in the form FID files which are impossible to understand without plotting. The raw data in the form of FID files was plotted using software BRUKER TOPSPIN which is presented in the form of images. The FID files are shared as supplemental files.

- Table 1 illustrate the rheological data of native and quaternized *Cassia tora* gum

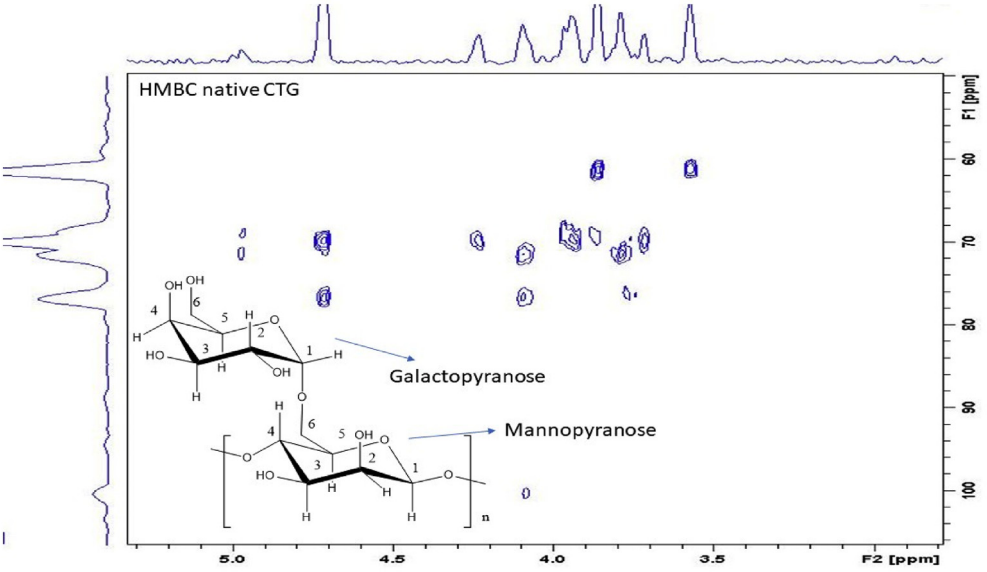

Fig. 4. HMBC spectra of native *Cassia tora* gum.

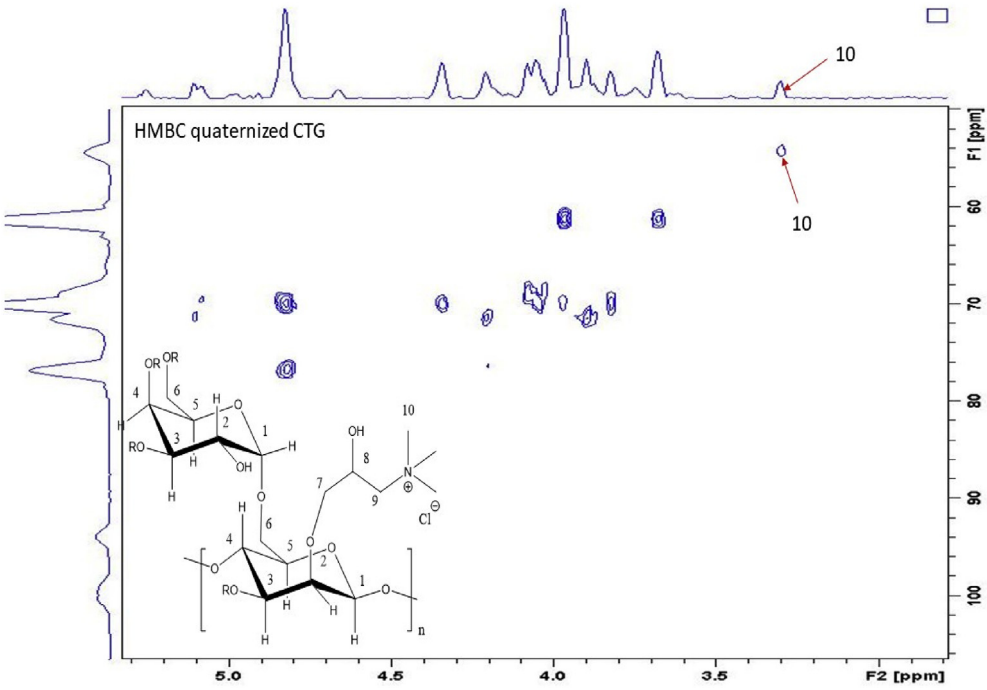

Fig. 5. HMBC spectra of quaternized *Cassia tora* gum.

Table 1
Rheological data of native and modified *Cassia tora* gum, Spindle-21, at Temperature-25 °C.

CTG			QCTG			
Shear rate (Sec^{-1})	3 hrs	24 hrs	3 hrs	24 hrs	48 hrs	120 hrs
Viscosity (cps) (2% solution)						
3.4	164.0	Degradation	424.1	389.0	414.8	370.2
6.8	147.6		384.3	351.5	366.7	311.4
17.0	130.8		331.8	300.9	306.0	249.3
34.0	114.8		280.4	250.1	252.7	209.0

2. Experimental design, material and methods

2.1. Collection of plant material

The plant material (dried legumes from the plant) was collected in the month of November from the surrounding area of Forest Research Institute, Dehradun, India. The legumes (Fig. 1 a) were sun dried and the seeds (Fig. 1 b) were separated manually from the legumes. Endosperm (Fig. 1 c) was separated from the seeds and powdered (Fig. 1 d). The quaternisation reaction was carried out on the endosperm powder to obtain the quaternized product (Fig. 1 e).

2.2. ^{1}H NMR spectroscopy

The ^{1}H NMR spectra of CTG and QCTG were acquired using a 500MHz Bruker spectrometer at 25°C. The samples were hydrolysed prior to recording the spectra [2]. *Cassia tora* gum (0.5 g) was added to aqueous sulphuric acid solution (20%, 50 mL) and stirred for 30 min at 50°C. After cooling at ambient temperature, the reaction mixture was neutralized by saturated sodium bicarbonate solution and dialyzed against deionised water for 48 hrs. The dialysate was filtered and freeze-dried. The freeze-dried sample (60 mg) was dissolved in D_2O (1 mL) for NMR spectral analysis.

2.3. Determination of rheological properties of native and quaternized CTG

The rheological properties were determined using Brookfield DV-III Ultra Digital Viscometer at 25 ± 1°C. The spindle-21 was used at a shear rate of 3.4, 6.8, 17.0 & 34.0 sec^{-1}.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2020.105271.

References

[1] D. Sharma, V. Kumar, R. Nautiyal, P. Sharma, Synthesis and Characterization of Quaternized *Cassia Tora* Gum Using Taguchi L'16 Approach, Carbohydrate Polymers, 2019, p. 115731.
[2] T. Muschin, T. Yoshida, Structural analysis of galactomannans by NMR spectroscopy, Carbohydr. Polym. 87 (3) (2012) 1893–1898.