

# NMR-BASED METABOLIC PROFILING OF EXTRACTS OF CINNAMON BUDS AND BARK



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**Introduction.** Cinnamon is one of the most popular spices used worldwide for cooking, but also in traditional and modern medicines for its beneficial properties. *Cinnamomum zeylanicum* and *Cinnamomum cassia* are the most important species. The most used part of cinnamon tree is the bark, but also the buds are used in the oriental culture. The metabolic profiles of aqueous/alcoholic extracts of cinnamon buds were characterized for the first time by NMR and compared with those of bark.



***C. zeylanicum* Bark (CZ)**  
True or Ceylon cinnamon



***C. cassia* Bark (CC)**  
Chinese cinnamon



***C. cassia* Buds (BC)**  
Unopened sun-dried flowers

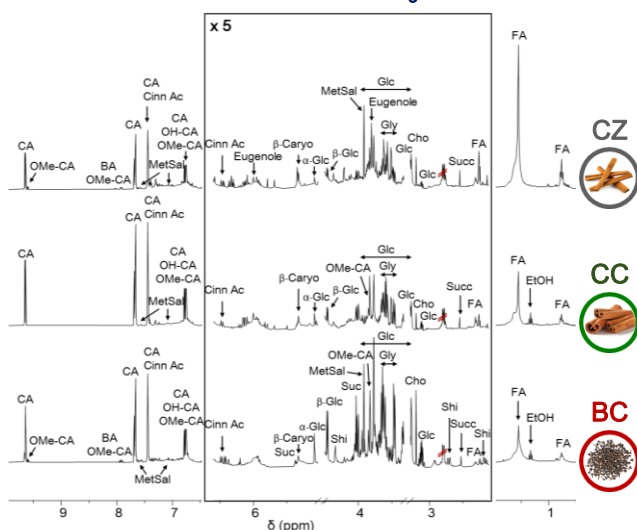


**Ultrasound extractions:**

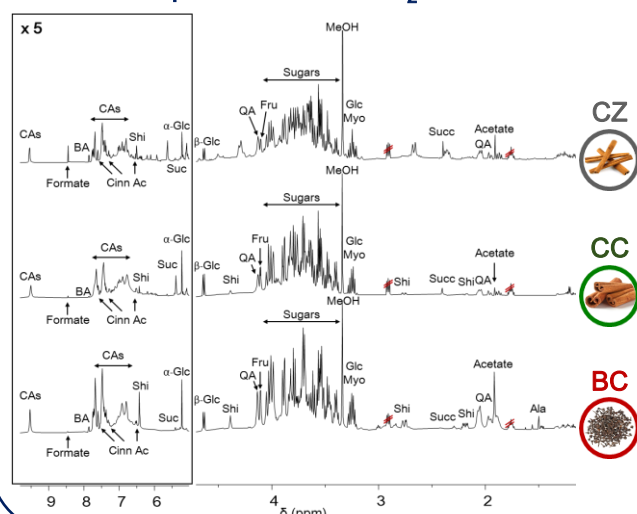
- Alcoholic (EtOH)
- Hydroalcoholic (H<sub>2</sub>O pH 4.5 / EtOH 7:3)
- Aqueous (H<sub>2</sub>O pH 4.5)

**NMR-based metabolic profiling of cinnamon extracts.** The metabolic profiles of cinnamon buds and bark extracts from different species (*C. cassia* and *C. zeylanicum*), obtained with different extraction solvents (ethanol, acid water/ethanol 7:3 and acid water) and dissolved both in CD<sub>3</sub>OD and D<sub>2</sub>O were characterized by NMR.

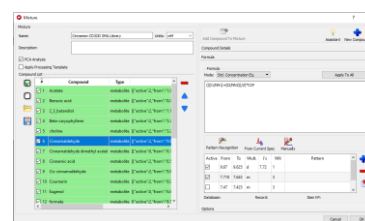
## Alcoholic extracts in CD<sub>3</sub>OD



## Aqueous extracts in D<sub>2</sub>O

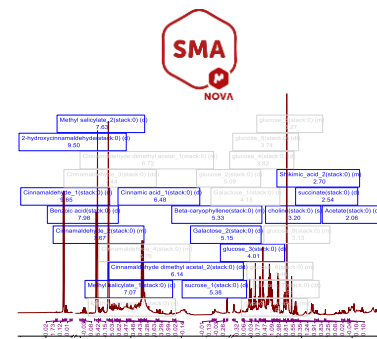


An NMR-based protocol for the rapid and semi-automatic identification and quantification of metabolites present in both cinnamon buds and bark extracts was developed, using the Simple Mixture Analysis (SMA) tool of MestReNova software, and specific metabolites' libraries were built up [1]. This procedure allows a considerable reduction in the time required for spectra analysis and determination of metabolites' concentration.



## SMA Library

Building of libraries for the food matrix of interest, available as .exp files [1].



## SMA assignment report

Simultaneous assignment of resonances on several <sup>1</sup>H-NMR spectra

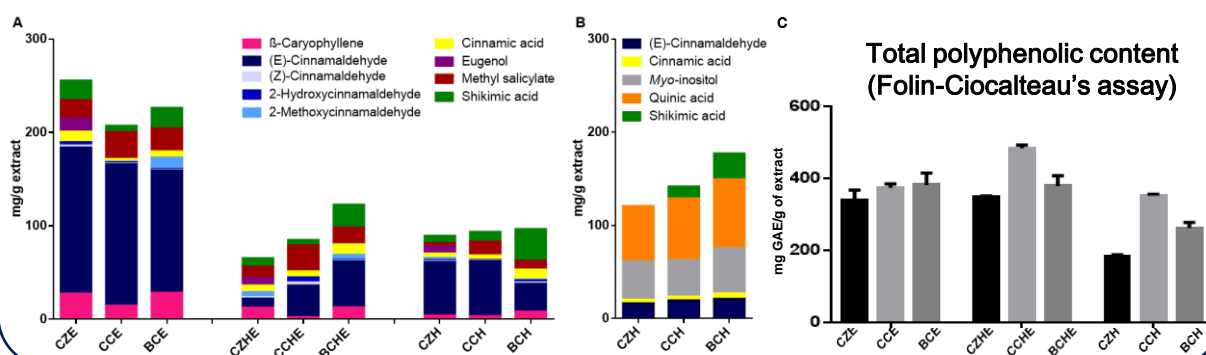
Metabolite	1	2	3
Acetic acid	3.00e-1	3.10e-1	7.02e-1
Benzoic acid	1.50e-1	4.00e-1	8.80e-2
2,3-Butanediol	1.80e-1	2.00e-1	2.27e-1
Beta-caryophyllene	8.80e-1	1.00	2.11
Choline	2.20e-1	7.02e-1	2.00e-1
Cinnamyl alcohol	1.50e-1	1.50e-1	1.50e-1
Cinnamyl alcohol	1.50e-1	1.50e-1	1.50e-1
Cinnamyl alcohol	1.50e-1	1.50e-1	1.50e-1
Cinnamyl alcohol	1.50e-1	1.50e-1	1.50e-1

**SMA concentration table**  
Simultaneous quantification of metabolites from different <sup>1</sup>H-NMR spectra

		mg/g of extract											
BC extract in		Benzoic acid	β-caryophyllene	Choline	Cinnam aldehyde	Cinnamic acid	Cis-cinnam aldehyde	Glucose	2-hydroxy-cinnam aldehyde	2-methoxy-cinnam aldehyde	Methyl salicylate	Shikimic acid	Sucrose
EtOH	M	1,91	28,29	1,42	130,93	6,75	0,94	93,96	0,84	11,94	24,75	21,74	9,24
	SD	1,32	8,7	0,5	7,09	5,6	0,21	21,97	0,3	1,66	1,82	12,33	8,22
H <sub>2</sub> O/ EtOH	M	0,65	12,65	2,31	49,31	11,24	0,61	72,62	0,89	5,46	17,99	24,5	6,18
	SD	0,84	3,23	0,8	15,29	4,85	0,26	21,11	0,88	1,96	1,82	12,56	4,4
H <sub>2</sub> O	M	0,55	8,02	2,79	29,96	10,62	1,51	88,96	2,04	0,89	9,75	33,63	7,69
	SD	0,41	0,33	0,07	8,41	2,27	0,96	1,94	1,33	0,58	1,88	2,97	1,52

[1] C. Airoidi, C. Ciaramelli, A. Palmioli (2021), "SMA libraries for metabolite NMR-based identification and quantification in cinnamon extracts", Mendeley Data, V1, doi: 10.17632/v3kj6zn9tf.1

**Healthy properties.** The content of bioactive compounds in CD<sub>3</sub>OD (A) and D<sub>2</sub>O (B) and the antioxidant activity (C) of cinnamon was evaluated, depending on starting material (buds or bark) and extraction (alcoholic E; hydroalcoholic HE; aqueous H).



## Conclusions

- The metabolic profile of cinnamon buds was characterized by NMR and compared to those of bark extracts
- Alcoholic extracts contained the highest amount of bioactive compounds
- Bud extracts content of healthy molecules was similar to bark ones
- The data collected provide useful insights for the selection of cinnamon raw material for preparation of dietary supplements and nutraceuticals