

Understanding the seasonal effect of metabolite production in *Terminalia catappa* L. leaves through a concatenated MS- and NMR-based metabolomics approach

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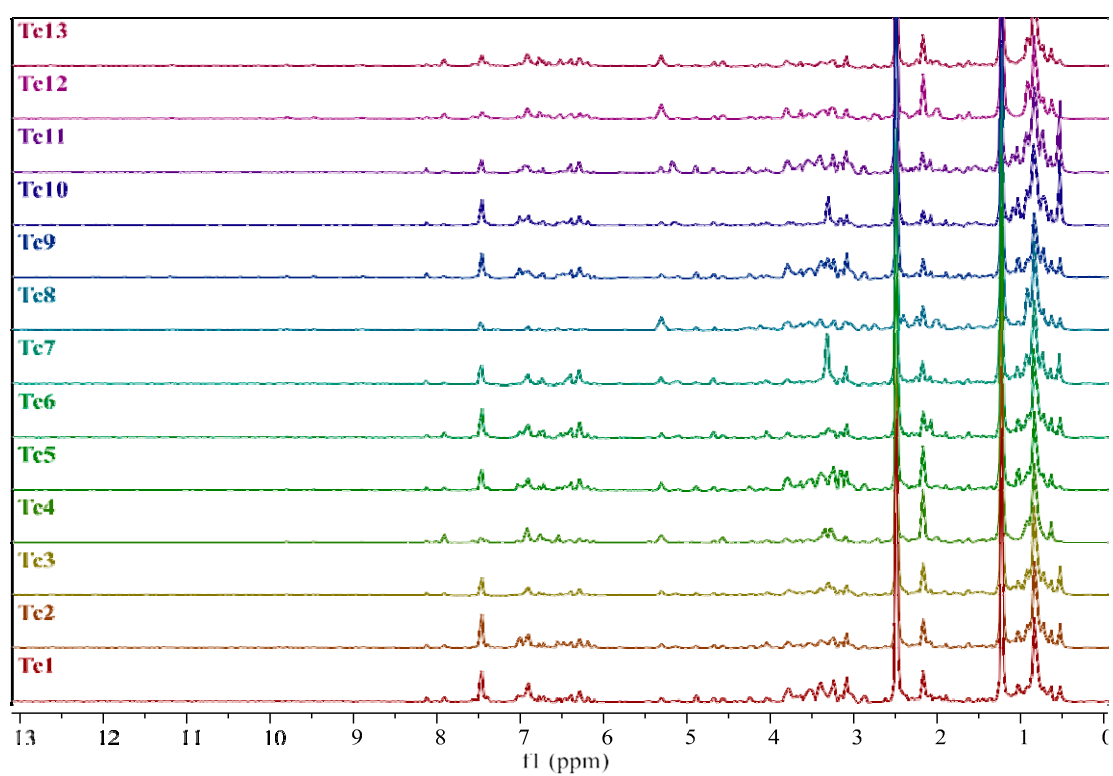


Figure S1. One-dimensional *J*-resolved NMR spectra (DMSO-*d*₆, 500 MHz) of *Terminalia catappa* samples (Tc1 to Tc13).

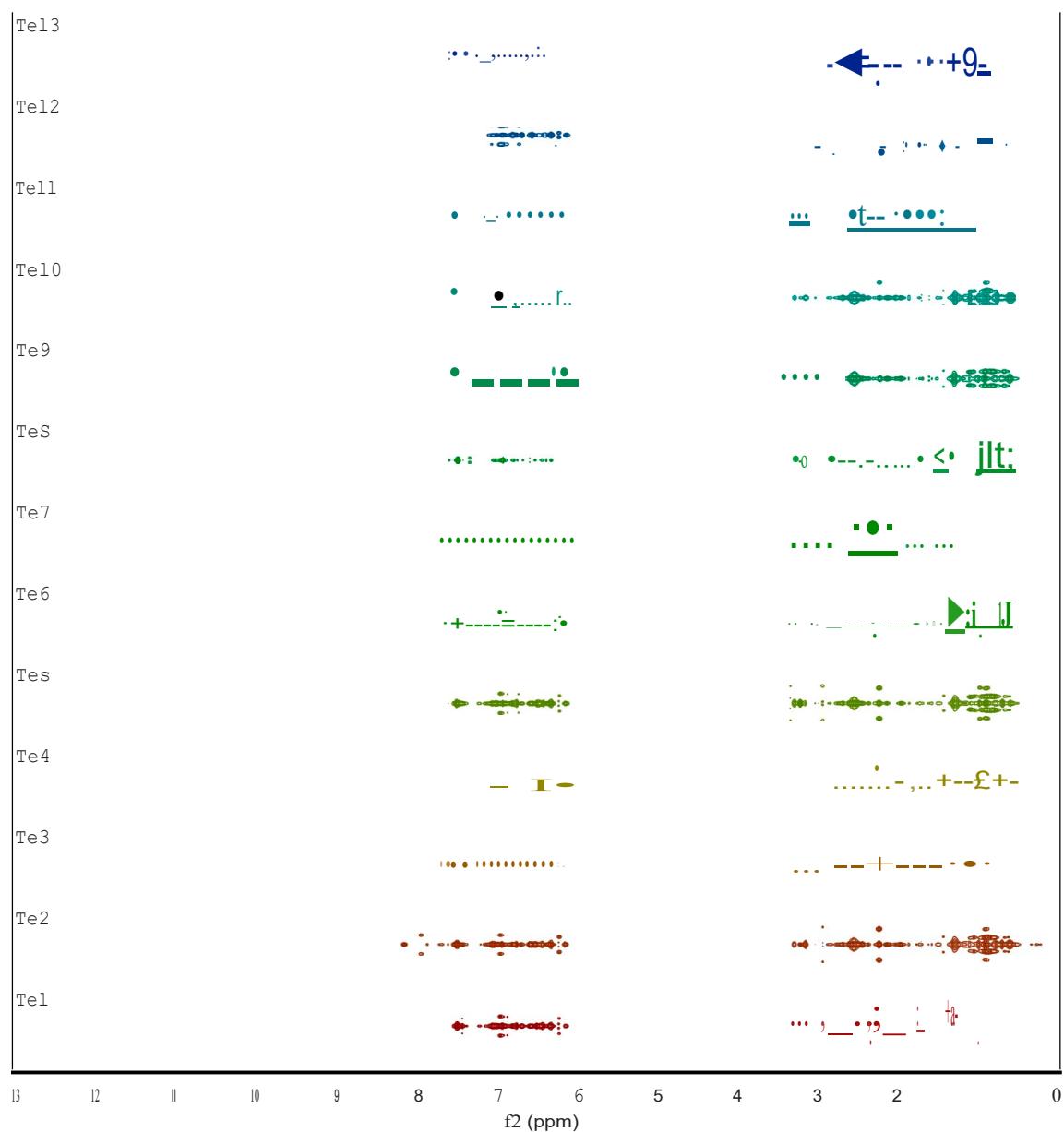


Figure S2. Two-dimensional J -resolved NMR spectra (DMSO- d_6 , 500 MHz) of *Terminalia catappa* samples (Tc1 to Tc13).

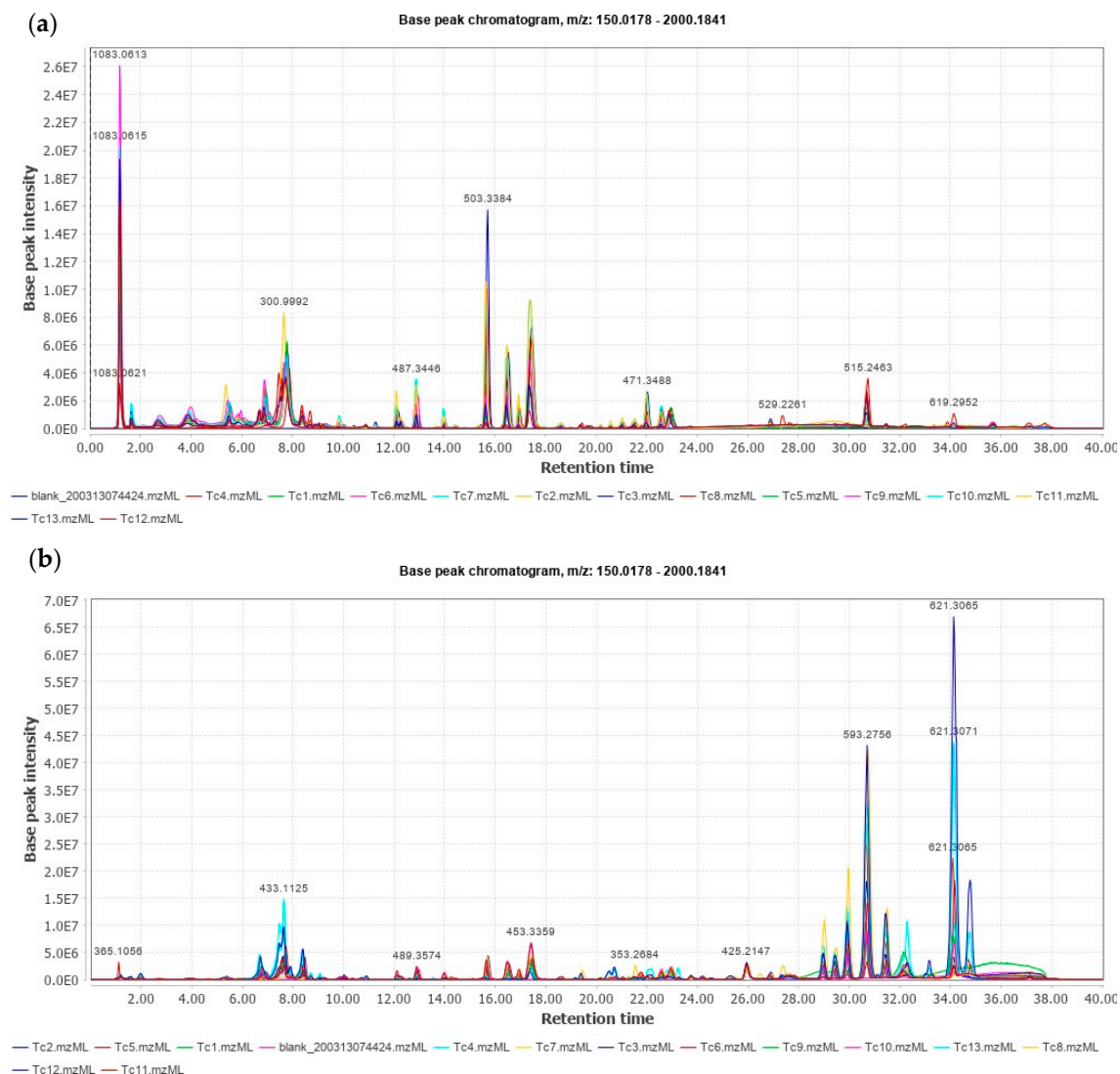


Figure S3. Base peak chromatogram for *Terminalia catappa* samples obtained from pre-processing by MZmine2: (a) negative ionization mode; (b) positive ionization mode.

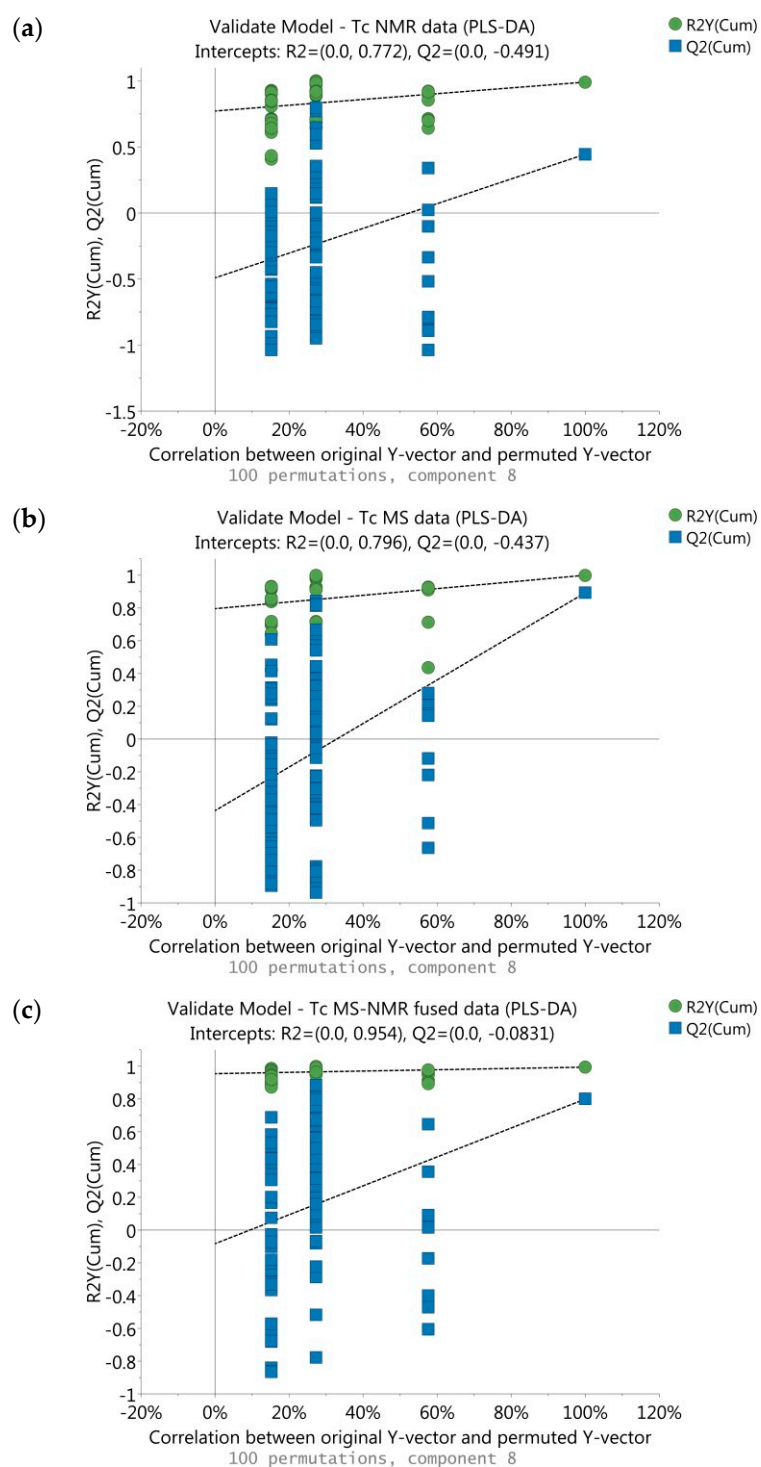


Figure S4. Permutation plot ($n = 100$ permutations) of PLS-DA validated model for *Terminalia catappa*: (a) NMR data; (b) MS data; (c) MS-NMR fused data.

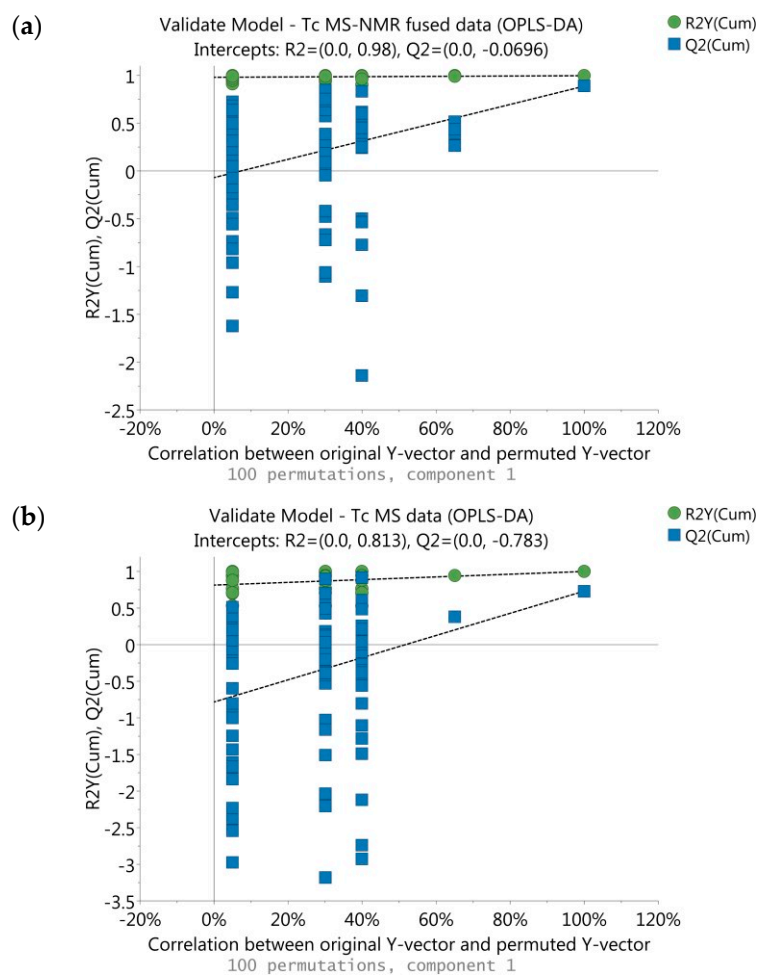


Figure S5. Permutation plot ($n = 100$ permutations) of OPLS-DA validated model for *Terminalia catappa*: (a) MS-NMR fused data; (b) MS data.

Supplementary Tables

Table S1. Weather characteristics for Santos-SP in 2017 and 2018: average temperature, solar radiation, air humidity and rainfall.

Period	Average of temperature (°C) per month	Average of solar radiation (kJ/m ²) per month	Average relative air humidity (%)	Cumulative amount of rainfall (mm) per month
Feb/17	29.4	2503.34	61	0.10
May/17	23.9	1551.68	70	0.19
Jun/17	23.1	1324.92	72	0.26
Aug/17	22.2	988.16	66	0.22
Oct/17	24.7	1079.44	75	0.19
Dec/17	25.2	771.04	84	0.43
Feb/18	30.4	901.93	75	0.60
Apr/18	27.4	931.46	70	0.38
Jun/18	24.6	1504.56	73	0.20
Jul/18	16.5	166.82	96	0.10
Aug/18	21.4	782.68	59	0.10
Oct/18	20.9	508.83	95	0.38
Nov/18	26.3	903.74	81	0.41

* The meteorological data were provided by the Meteorological Data Storage Section (SADMET) of the National Institute of Meteorology (INMET). Accessed at: www.inmet.gov.br.