

Supplementary Materials

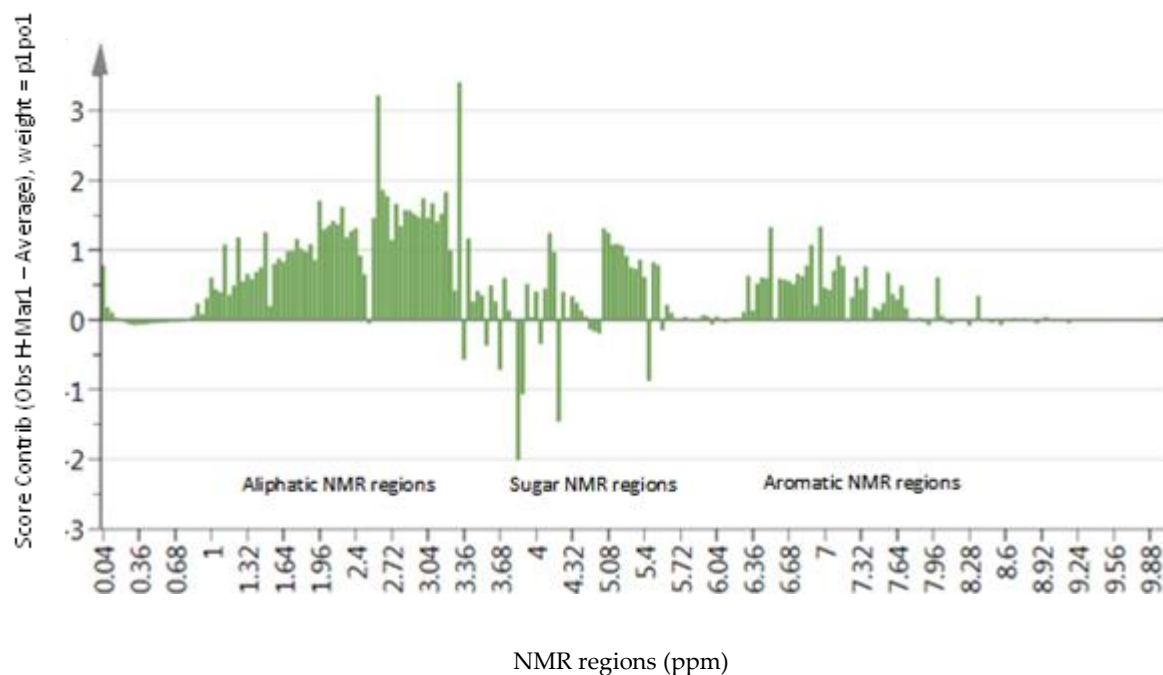


Figure S1. Contribution plot showing metabolites peaks in the NMR aliphatic, sugar and aromatic regions of *M. oleifera* leaf metabolomics associated with March sample separation under high harvesting frequency as shown in Figure 2.

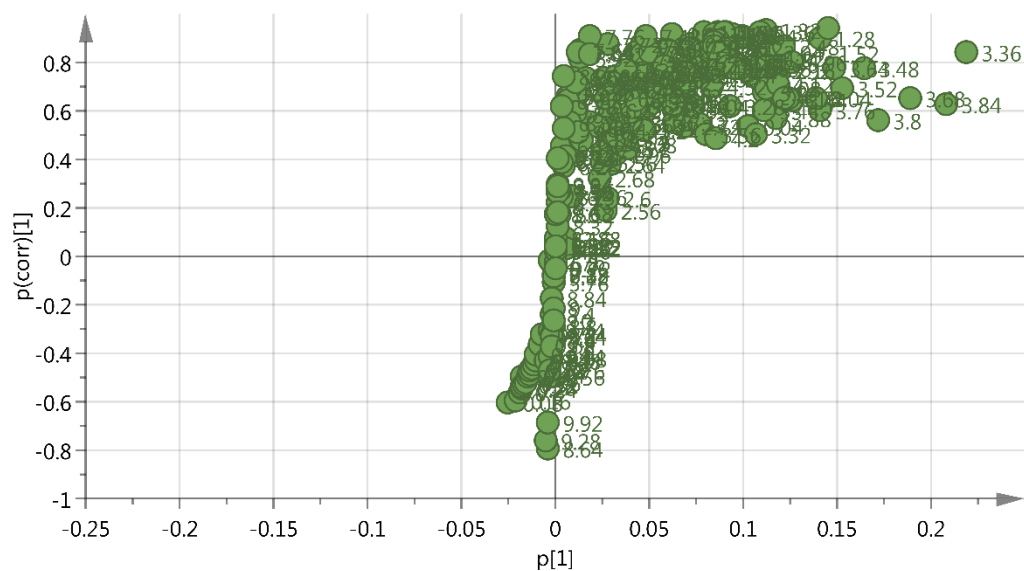


Figure S2. OPLS-DA loading score plot showing ^1H NMR spectral data of *M. oleifera* (cultivar PKM1) metabolite profile under low/ intermediate and high harvesting frequency ($R^2X[1] = 0.472$; $R^2Xo[1] = 0.358$)

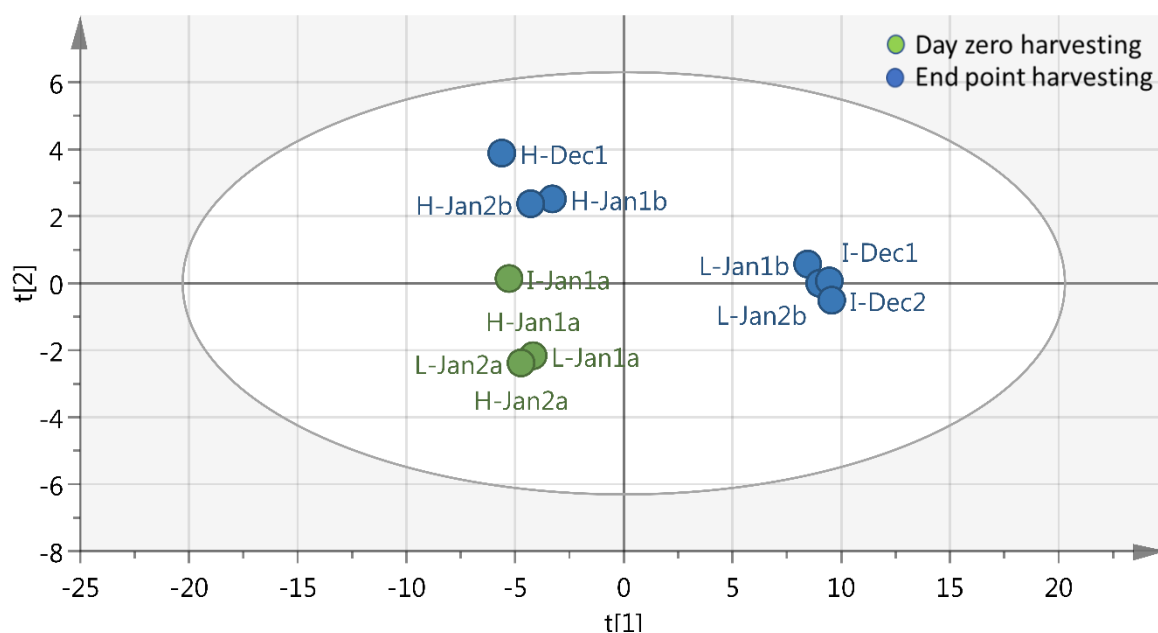


Figure S3. PLS-DA score plot showing ^1H NMR spectral data of *M. oleifera* (cultivar PKM1) metabolite profile under low/ intermediate and high harvesting frequencies, showing separation between day 0 and end point harvesting ($R^2X = 0.954$; $R^2Y = 0.93$; $Q^2 = 0.902$). H-Jan = high frequency; I-Jan = intermediate frequency; L-Jan = low frequency. $R^2X[1] = 0.88$; $R^2X[2] = 0.0746$

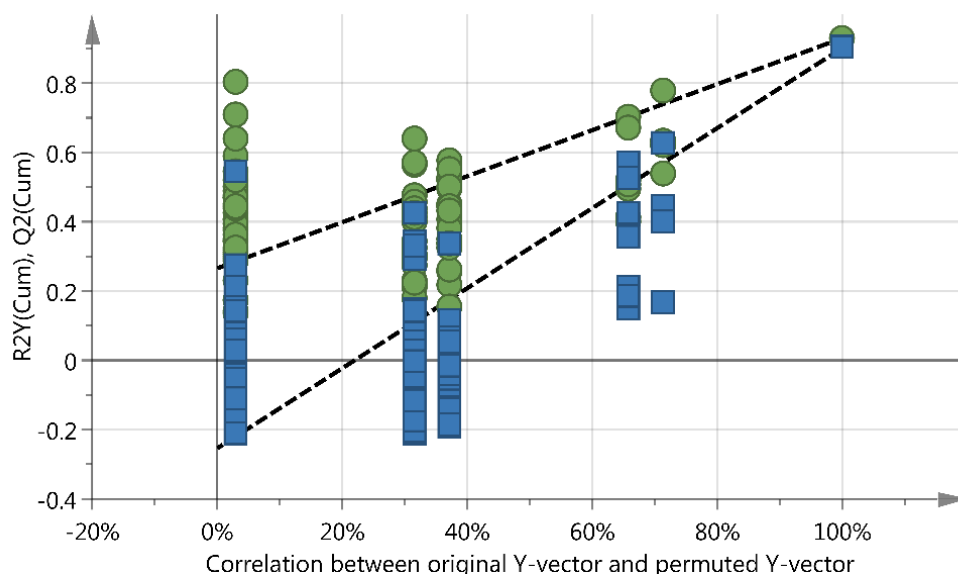


Figure S4. PLS-DA model validity permutation test for *M. oleifera* (cultivar PKM1) metabolite profile under low, intermediate and high harvesting frequencies. ($R^2X = 0.954$; $R^2Y = 0.93$; $Q^2 = 0.902$). $R^2 = (0.0; 0.266)$, $Q^2 = (0.0, -0.254)$

Table S1 ¹H-NMR spectral regions of annotated compounds that contributed to the separation of leave samples.

Treatment	Compounds	¹ H-NMR Chemical shifts (ppm)	Referenced chemical shifts (ppm)	References	Chenomx (ppm)	Assigned numbers
Low and intermediate harvesting frequency	Ferulic acid	6.38, 6.86, 7.05 7.33	6.388, 6.86, 7.05, 7.3	(Anselmi et al., 2006) https://hmdb.ca/spectra/nmr_one_d/1934 (HMDB accessed 16.08.2020)	6.4, 6.9, 7.1	1
	Chlorogenic acid	2.02, 2.17, 6.39, 7.05, 7.15, 7.64	2.02, 2.18, 6.39 7.05, 7.14, 7.63	https://hmdb.ca/spectra/nmr_one_d/1934 (HMDB accessed 16.08.2020) (Sabino et al., 2019)	6.4, 6.9, 7.1 7.6	2
	Vanillic acid	6.94, 7.55, 7.65	6.93, 7.54, 7.64	https://hmdb.ca/spectra/nmr_one_d/1390 (HMDB accessed 16.08.2020) (Sakushima et al., 2003)	6.9, 7.4, 7.5	3
	Niazirin	1.2, 3.84, 7.16, 7.26	1.21, 3.81, 7.2, 7.26	(Faizi et al., 1994; Gilani et al., 1994; Maurya et al., 2011)		4
	Esculetin	3.21, 3.35, 7.42, 7.55	3.21, 3.35, 7.4 7.5	(Aboul-Ela et al., 2002)		5
	Wogonin	3.86, 6.3, 7.09, 7.59	3.86, 6.32, 7.09 7.67	(Jang et al., 2005; Li et al., 2009)		6
	GABA	1.9, 2.3, 3.01	1.88, 2.28, 3.01	(Kaiser et al., 2008)	1.9, 2.3, 3.0	7