**Supporting Information**

**Multipronged Approach to Profiling Metabolites in *Beta Vulgaris* Dried Pulp Extract Using Chromatography, NMR, and other Spectroscopy Methods**

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Figure S1. COSY spectrum showing the amino acid Leucine (D2O-salt, 400 MHz).

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Figure S1. COSY spectrum showing the amino acid Leucine.

![Chart, histogram

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Figure S2. MS spectra of 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z) (RT = 10.846 min.) experiment spectrum overlaid with the reference library spectrum.

![Chart, bar chart, histogram

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Figure S3. MS spectra of 9-Octadecenoic acid, methyl ester, (E) (RT = 10.027 min.) experiment spectrum overlaid with the reference library spectrum.

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Figure S4. MS spectra of methyl stearate (RT = 9.927 min.) experiment spectrum overlaid with the reference library spectrum.

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Figure S5. MS spectra of hexadecanoic acid, methyl ester (RT = 8.411 min.) experiment spectrum overlaid with the reference library spectrum.



Figure S6. Proton-decoupled 31P NMR spectra of polar extract (A) in D2O and non-polar extract (B) in CDCl3 on a 400 MHz spectrometer, ns = 10,000 at 25°C temperature, and 20 Hz line-broadening. Chemical shift is based on the 31P peak of 85% phosphoric acid, which is set at 0 PPM.

Figure S6 shows the proton-decoupled 31P spectra of the polar extract in D2O (A) and non-polar extract in CDCl3 (B). The chemical shift of 31P peaks in both media falls between 0 and 6.5 PPM. The peaks were then assigned to orthophosphate monoester (polar phase), and to orthophosphate diester (non-polar phase)[1]. It is interesting to note that no 31P signals were observed in the middle layer that we obtain during extraction: The middle layer contains molecules that are not soluble in H2O/methanol or CHCl3. This suggests that phosphorus compounds (mono- and di-ester orthophosphate) split during the extraction between the polar and non-polar phases according to their polarity and the polarity of the phase.

References

[1] B. J. Cade-Menun, “Improved peak identification in 31P-NMR spectra of environmental samples with a standardized method and peak library,” *Geoderma*, vol. 257–258, pp. 102–114, 2015.