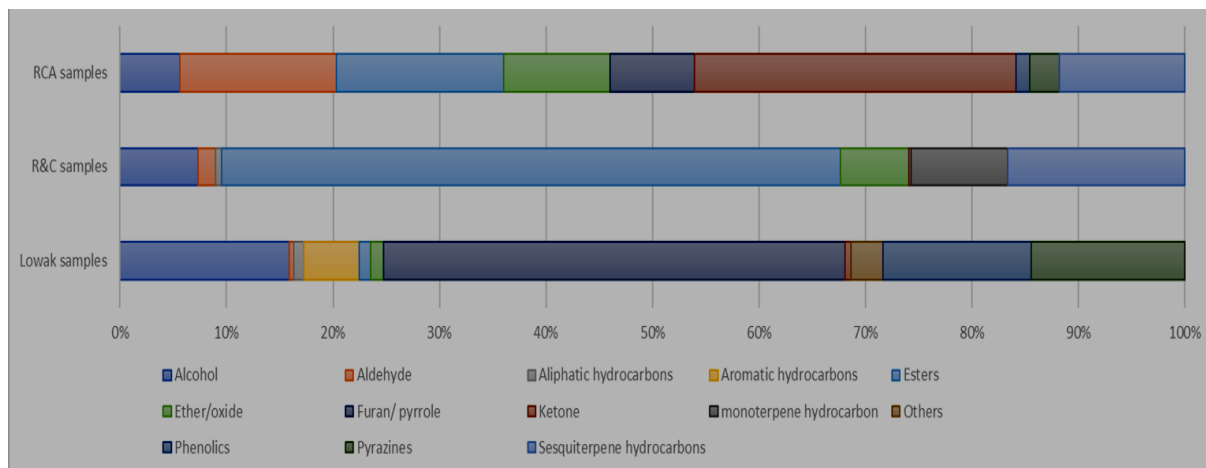
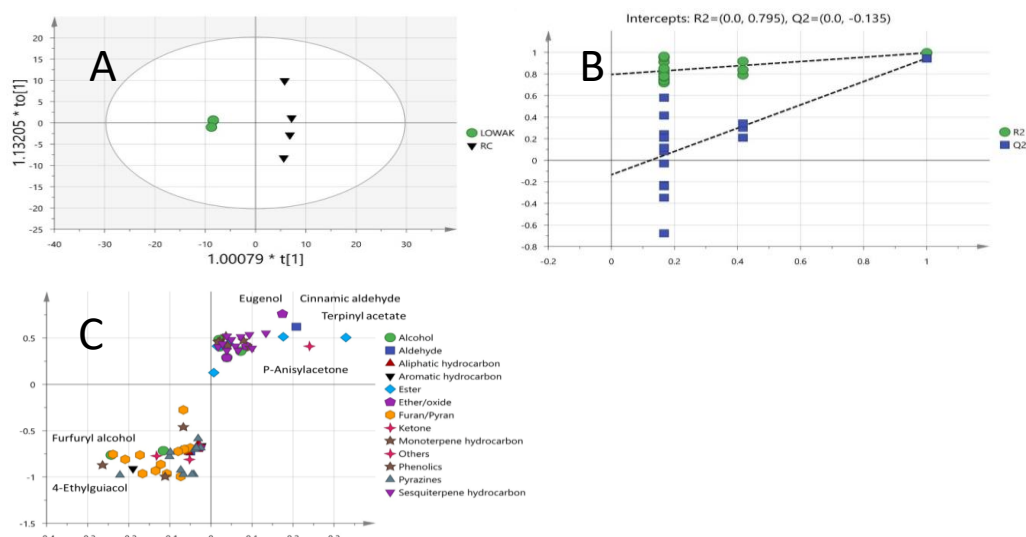


Suppl. Figure S1 (A) HSQC NMR spectra for assignment of 1, sucrose; 2, 5-CQA; 3, 4-CQA; 4, trigonelline; 5, caffeine; 6, quinic acid (B) HSQC NMR spectra for assignment of caffeoyl shikimic acid (C, D) HSQC and HMBC NMR spectra for assignment of octadec-9-enoic acid as a major fatty acid constituent in Luwak coffee seeds. (E) HSQC NMR spectra for assignment of Nitrogen compounds (Caffeine and

trigonelline) (F) HMBC NMR spectra for assignment of n-methylpyridinium. All assignment details are listed in Table 1



Suppl. Figure S2 Percentile proportion of metabolite groups in different coffee samples as identified by SPME/GC-MS



Suppl. Figure S3 (A) OPLS-DA model score plot of Luwak coffee versus roasted coffee, (B) Permutation analysis to validate OPLS-DA model score plot of Luwak coffee versus roasted coffee, (C) OPLS-DA model S-plot of Luwak coffee versus roasted coffee