This is an excellent manuscript, and should certainly be published in the journal without significant changes.

A few points the authors might want to consider:

1. The samples include brews prepared from 100% arabica beans, and samples prepared from arabica–robusta blends, but no samples prepared 100% robusta beans. If 100% robusta samples had been included in the sample set, this should have resulted in greater statistical discrimination of those metabolites referred to in Figure 3, and to an even better resolution of PCA scores subpopulation clusters shown in Figure 1B. The reviewer does not mean to suggest here that the subpopulation resolution in Figure 1B is not convincing, because it certainly is, but simply that an even better resolution would be obtained if 100% robusta samples were included in the sample set. However, the sample population examined in this study specifically targets coffee brews that are actually consumed by the coffee drinking population in the United States. It seems possible that no 100% robusta brews are actually drunk in United States. Still if this is in fact the case the authors might want to include a sentence clarifying the situation.

   **Reply:** *This is indeed the case. There are no commonly consumed 100% Robusta coffees in the US to the best of our knowledge. A sentence has been added (line xxx).*

2. Do the authors know the percentage by weight of the arabica and robusta beans present in the blend samples? Does this percentage vary in commercially available blended coffee brews in the United States? In this study was this percentage constant over the sample set? If this information is available, the authors might want to include it in a brief sentence or two in the manuscript.

   **Reply:** *The exact mixtures are not disclosed by the food manufacturers, and it is difficult to find reliable information on the ratios. Generally speaking blends seem to have no more than 20% Robusta (with 80% arabica) due to the bitterness of the Robusta beans. A sentence has been added (line xxx).*

3. In describing the sample set on line 213 the authors refer to three roast levels, “light”, “medium” and “dark”. However in Figure 3 only data from the “medium roast” and “dark roast” subpopulations are presented. What happened to the light roast samples? The authors might want to include a sentence clarifying the fate of the light roast samples.

   **Reply:** *Light roasted samples were not included in this analysis because of a too low number of samples (four samples prepared with different brewing methods).*

The manuscript is very well written, very clear as to intended meaning, and very readable through-out. Two minor points:

4. In line 22 the authors refer to “41% variability”. The reviewer believes that this should be “41% variance”.

   **Reply:** *This has been corrected (abstract).*
5. Throughout the manuscript the authors refer to the sample population in this study as derived from 74 coffee brew samples. In the abstract on line 15, and again in the section describing the Supplementary Materials on line 317, the authors refer to 76 coffee brew samples. Please clarify. Is this difference due to the two samples that were separated out from the population to be used for analytical method quality control?

Reply: Thank you for noting this error. The number is 76 and this has been corrected.