Supplementary Material

Microbial Interactions in Kombucha through the Lens of Metabolomics

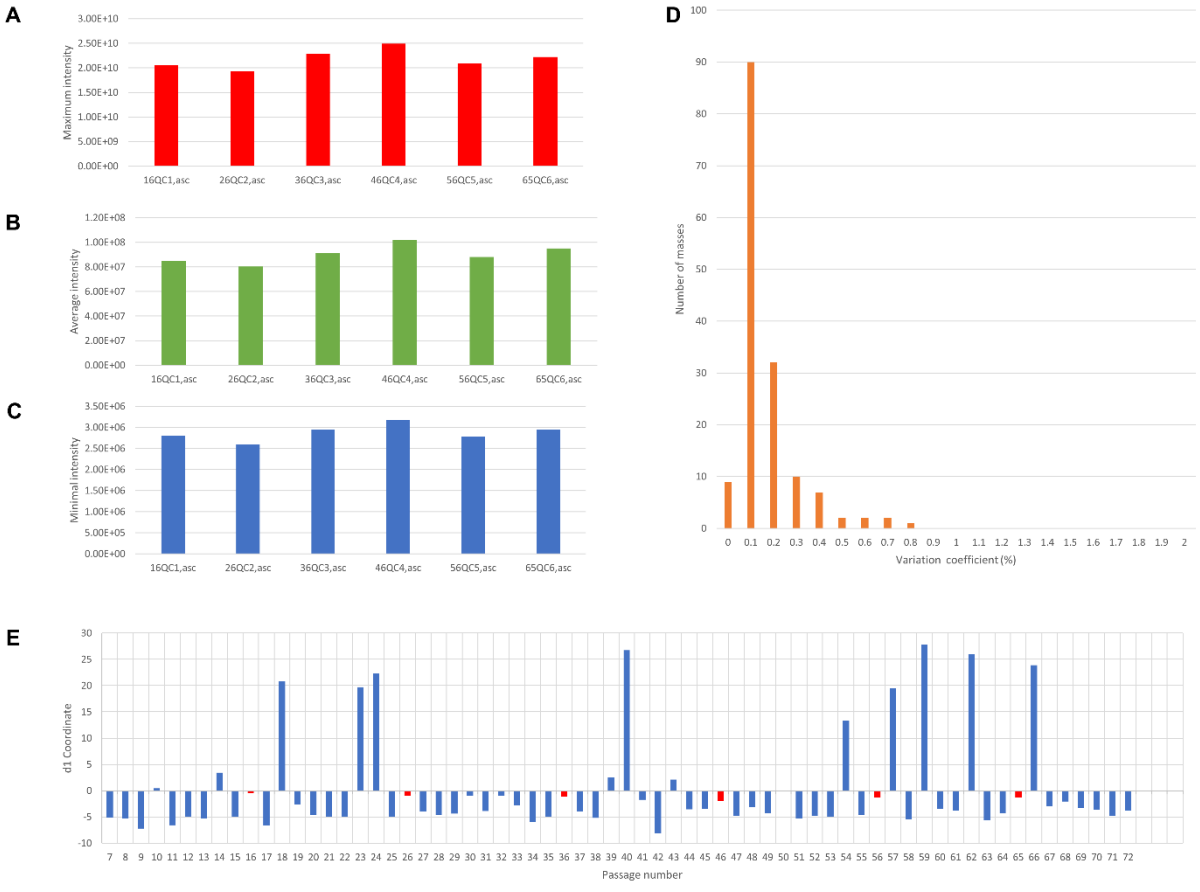

Figure S1: Visualization of Quality control (QC) samples. (A) maximum, (B) average and (C) minimal ion intensities measured in QC samples. (D) Distribution of mass number according to variation coefficient of QC samples. (E) Principal Component Analysis d1 coordinate of samples according to passage number, with QC samples signalized in red.

Table S1: Database annotation of markers

Mass (average)	Formula	Database annotation
163.04006	$C_9H_8O_3$	Phenylpyruvate
169.01427	$C_7H_6O_5$	Gallic acid
173.00917	$C_6H_6O_6$	aconitic acid
175.06121	$C_7H_{12}O_5$	Isopropyl malate
178.04774	$C_{10}H_6O_6$	Gluconolactone
179.05612	$C_6H_{12}O_6$	Glucose or Fructose
189.04046	$C_7H_{10}O_6$	Dehydroquinic acid
191.01973	$C_6H_8O_7$	Citric acid
195.05103	$C_6H_{12}O_7$	Gluconic acid
253.21727	$C_{16}H_{30}O_2$	Palmitoleic acid
255.23292	$C_{16}H_{32}O_2$	Palmitic acid
281.24859	$C_{18}H_{34}O_2$	Oleic acid
283.26424	$C_{18}H_{36}O_2$	Stearic acid
289.07175	$C_{15}H_{14}O_6$	Epicatechin
300.26645	$C_{18}H_{36}O_3$	Hydroxystearic acid
341.10891	$C_{12}H_{22}O_{11}$	Sucrose
441.08278	$C_{22}H_{18}O_{10}$	Epicatechin gallate
503.16189	$C_{18}H_{32}O_{16}$	Dextrin
535.15180	$C_{18}H_{32}O_{18}$	1,4-bêta-D-Glucan

Figure S2: Distribution of annotated compounds using MASSTRIX database according to metabolic pathways according to KEGG Mapper Color.

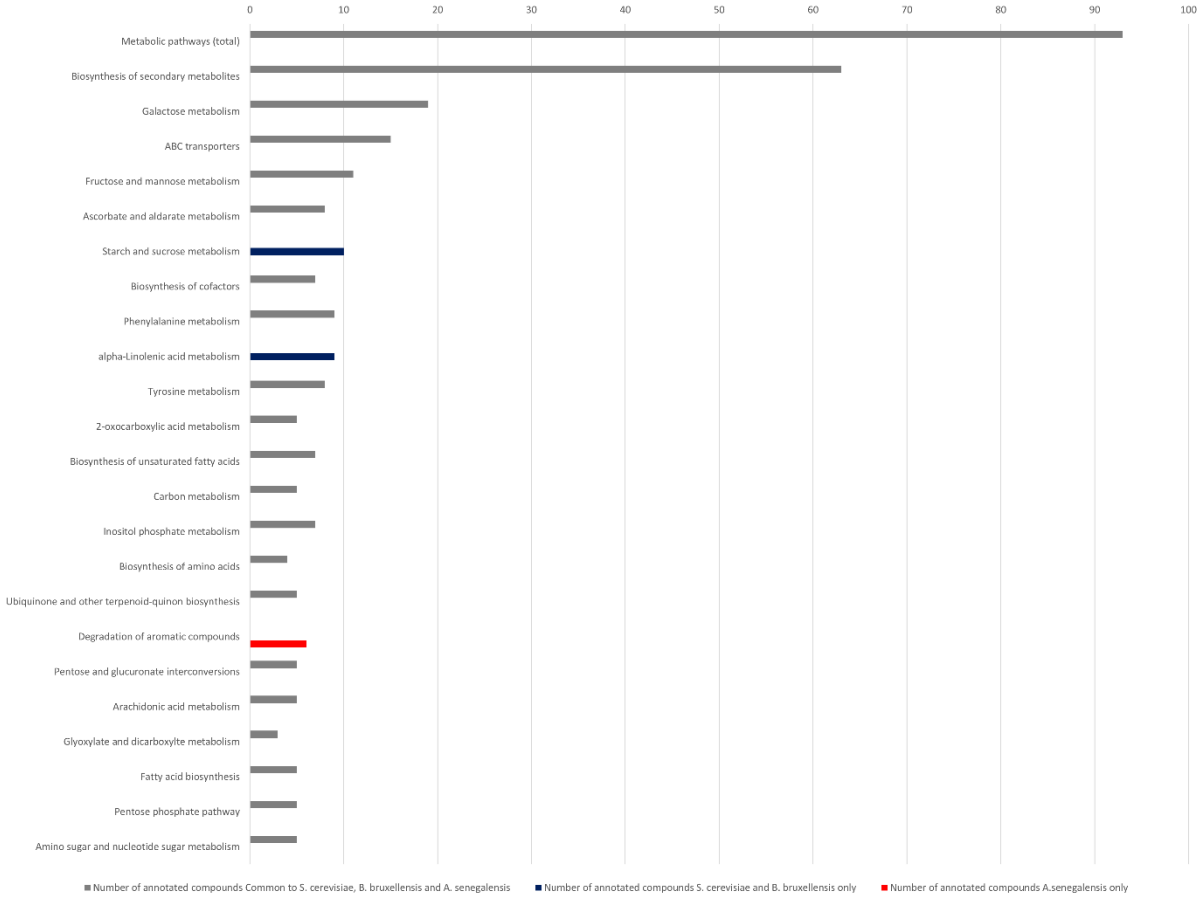

Figure S3: Venn diagram showing the number of common and unique formulae between those produced in BBHV as part of the interaction between *B. bruxellensis* (BB) and *H. valbyensis* (HV) (labeled "BBHV(BBHV)" and those present in BBHV but inhibited by the presence of *A. indonesiensis* (AI) in the coculture gathering all three microorganisms (T) (labeled "BBHV(T)").

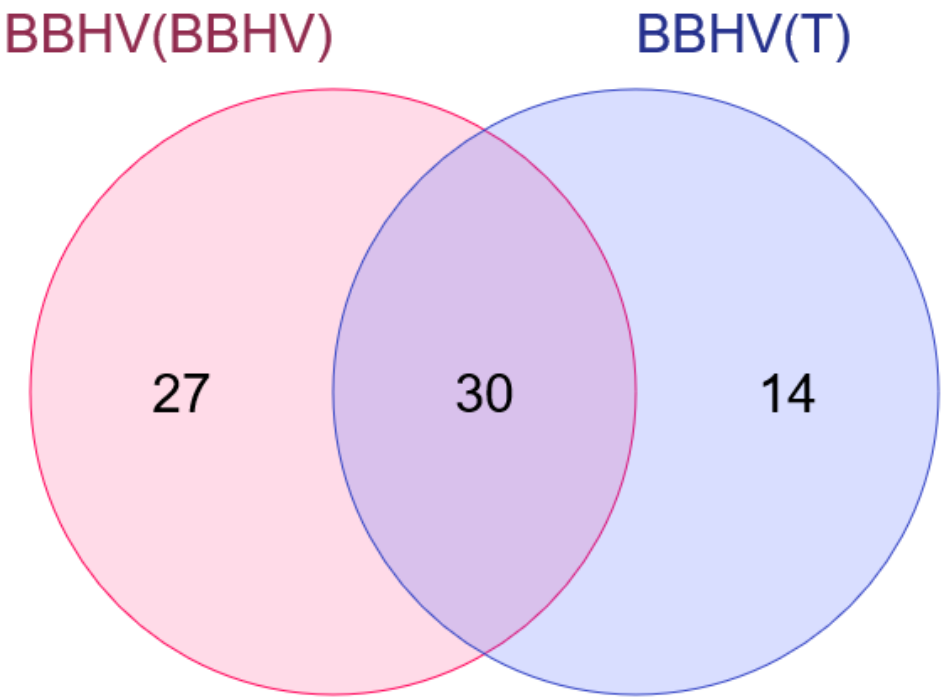

Figure S4: Venn diagram showing the number of common and unique formulae between the lists of those associated with *A. indonesiensis* monoculture (AI), that were negatively impacted by the presence of yeast(s). The three cases involved *B. bruxellensis* alone (BBAI), *H. valbyensis* alone (HVAI) and the two yeasts simultaneously (T).