

Table 1. Biomarkers identified from redundancy analysis (RDA) of the effect of proxies of herbivory on natural log-transformed relative peak areas of volatile compounds detected in tea. Compounds are ordered by the absolute value of their correlation to the constrained RDA axis. For each compound, univariate tests were performed to test for a linear and step-function relationship. For the linear relationship, the slope coefficient is reported in units of ln(RPA) (i.e. not back-transformed) and the change point, “step”, is reported in units of leafhoppers / young leaf for the density biomarkers and in units of percent leaf damage for the damage biomarkers.

Herbivory proxy	Compound	CAS	Multivariate			Univariate			Aroma	Chemical Family
			RDA axis loading	Correlation to RDA axis	Correlation p-value	Slope	Linear regression p-value	Change point		
Leafhopper density	(E,E)- $\alpha$ -Farnesene	502-61-4	-0.271	-0.811	< 0.001	6.400	0.001	0.333	woody, sweet, green, floral	Sesquiterpene
	Sulcatone	110-93-0	-0.210	-0.794	< 0.001	2.212	0.021	0.625	green, musty, pepper, mushroom, rubber	Aliphatic ketone
	$\beta$ -Myrcene	123-35-3	-0.244	-0.761	< 0.001	1.336	0.006	0.682	balsamic, must, spice	Monoterpene
	(E)- $\beta$ -Ocimene	3379-61-1	-0.223	-0.730	< 0.001	5.227	0.012	0.167	citrus, green, terpene	Monoterpene
	trans- $\alpha$ -Bergamotene	13474-59-4	-0.238	-0.685	0.001	1.923	0.006	0.500	woody, warm, tea	Monoterpene
	Indole	120-72-9	-0.157	-0.681	0.001	1.614	0.092		- concentrated = fecal, animal dilute = sweet, floral	Nitrogen containing
	(E,E)-Allo-ocimene	3016-19-1	-0.184	-0.668	0.002	1.867	0.044	0.167	terpenic, sweet, fresh, floral	Monoterpene
	cis-Butyric acid, 3-hexenyl ester	16491-36-4	-0.190	-0.649	0.003	1.941	0.038		- wine, green	Fatty acid ester
	Hexanoic acid	142-62-1	0.133	0.639	0.003	-2.236	0.116		- cheesy, fatty	Fatty acid
	(Z)- $\beta$ -Ocimene	3338-55-4	-0.155	-0.625	0.004	1.713	0.092	0.167	citrus, herbal, floral	Monoterpene
	trans-Dehydroxylinalool oxide	54750-70-8	-0.126	-0.620	0.005	0.751	0.125		- herbal, green, terpene	Oxygenated monoterpene
	Heptanoic acid	111-14-8	0.135	0.615	0.005	-2.037	0.116		- cheesy, sour, rancid	Fatty acid
	Octanoic acid	124-07-2	0.143	0.609	0.006	-2.367	0.109		- cheesy, fatty, waxy	Fatty acid
	2-Methyl-1H-pyrrole	636-41-9	-0.177	-0.579	0.009	0.907	0.051	0.500	-	Nitrogen containing
	24	-	-0.141	-0.575	0.010	0.846	0.109		- -	-
	(3Z)-Hexenyl hexanoate	31501-11-8	-0.140	-0.530	0.020	1.516	0.109		- fruit, prune	Fatty acid ester
	cis-Linalool oxide (pyranoid)	14009-71-3	-0.151	-0.525	0.021	1.494	0.096		- citrus, green	-
	$\gamma$ -Butyrolactone	96-48-0	0.120	0.520	0.022	-0.749	0.140		- caramel, fatty, sweet	Oxygenated heterocycle
	cis-Linalool oxide (furanoid)	5989-33-3	-0.131	-0.517	0.023	1.761	0.117		- earthy, floral, sweet, woody	Oxygenated heterocycle
	Diendiol I	13741-21-4	-0.203	-0.494	0.032	2.011	0.024	0.429	-	Oxygenated monoterpene
Focal leaf damage	1-Hexanol	111-27-3	0.212	0.830	< 0.001	0.096	0.041	4.206	resin, flower, green	Aliphatic alcohol
	(E)-2-Hexen-1-ol	928-95-0	0.230	0.783	< 0.001	0.093	0.041		- green, leaf, walnut	Alkenyl alcohol
	N,N-Dibutylformamide	761-65-9	0.168	0.703	0.001	0.078	0.077		- -	Nitrogen containing
	Benzothiazole	95-16-9	0.195	0.699	0.001	0.074	0.067		- rubbery, sulfury, vegetal, gasoline	Nitrogen sulfur containing
	(3Z)-Hexenyl hexanoate	31501-11-8	0.181	0.671	0.002	0.088	0.068		- fruit, prune	Fatty acid ester
	Phenethyl alcohol	60-12-8	0.212	0.671	0.002	0.119	0.041		- honey, spice, rose, lilac	Aromatic alcohol
	cis-3-Hexenyl isovalerate	35154-45-1	0.213	0.613	0.005	0.080	0.041	8.541	fresh, green, apple, fruity, tropical, pineapple	Fatty acid ester
	(3-hydroxy-2,4,4-trimethylpentyl), 2-methylpropanoate	74367-34-3	0.153	0.609	0.006	0.031	0.103		- -	Aliphatic ester
	cis-Butyric acid, 3-hexenyl ester	16491-36-4	0.182	0.604	0.006	0.083	0.068		- wine, green	Fatty acid ester
	2-Cyclopentene-1,4-dione	930-60-9	0.190	0.575	0.010	0.042	0.068		- -	Cyclic ketone
	Benzyl alcohol	100-51-6	0.168	0.561	0.012	0.070	0.077		- fruity, floral, sweet	Cyclic alcohol
	Phenylacetaldehyde	122-78-1	0.144	0.511	0.025	0.046	0.122		- floral, honey, sweet	Cyclic aldehyde
	o-Hydroxybiphenyl	90-43-7	0.119	0.505	0.027	0.037	0.182		- -	Aromatic compound
	Dodecanoic acid	143-07-7	0.136	0.473	0.041	0.083	0.141		- mild, fatty, coconut, bay oil, metal	-
	2,4-Di-tert-butylphenol	96-76-4	0.165	0.472	0.041	0.029	0.077		- -	-
	Tetradecanoic acid	544-63-8	0.123	0.466	0.044	0.041	0.179		- coconut, soapy, waxy	Fatty acid
	(Z)- $\beta$ -Ocimene	3338-55-4	-0.172	-0.466	0.044	-0.085	0.077		- citrus, herbal, floral	Monoterpene
	Mesityl oxide	141-79-7	0.049	0.459	0.048	0.012	0.585		- acrylic, earthy, sweet, chemical	Aliphatic ketone