

Table 1. Biomarkers of leafhopper density in order of the strength of correlation to the RDA constrained axis. For each compound, the type of univariate relationship between log transformed relative peak areas and leafhopper density is reported. For step function relationships, the change point is reported in units of leafhoppers per young leaf.

Compound	CAS	Multivariate		Univariate				
		RDA Loading	RDA Correlation	Response type	Linear Slope	Change point	ΔIntercept	Aroma
cis-Butyric acid, 3-hexenyl ester	16491-36-4	-0.185	-0.817***	linear	3.941	-	-	wine, green
(E,E)-α-Farnesene	502-61-4	-0.216	-0.814***	step	-	0.312	15.075	woody, sweet, green, floral
Sulcatone	110-93-0	-0.202	-0.804***	linear	4.11	-	-	green, musty, pepper, mushroom
(3Z)-Hexenyl hexanoate	31501-11-8	-0.169	-0.77***	step	-	0.579	10.444	green, fruity, fatty, tropical
3	-	-0.183	-0.755***	linear	2.293	-	-	-
(E)-β-Ocimene	3379-61-1	-0.195	-0.751***	step	-	0.25	14.521	citrus, green, terpene
trans-Dehydroxylinalool oxide	54750-70-8	-0.167	-0.741***	step	-	0.625	10.313	herbal, green, terpene
cis-Linalool oxide (pyranoid)	14009-71-3	-0.175	-0.717***	step	-	0.429	9.876	citrus, green
cis-Linalool oxide (furanoid)	5989-33-3	-0.158	-0.713***	linear	3.65	-	-	earthy, floral, sweet, woody
(E,E)-Allo-ocimene	3016-19-1	-0.175	-0.684**	step	-	0.25	10.159	terpenic, sweet, fresh, floral
Indole	120-72-9	-0.141	-0.669**	step	-	0.682	7.266	concentrated = fecal, animal dilute = sweet, floral
Diendiol I	13741-21-4	-0.185	-0.668**	linear	3.673	-	-	-
Benzyl alcohol	100-51-6	-0.155	-0.66**	linear	2.276	-	-	fruity, floral, sweet
β-Myrcene	123-35-3	-0.154	-0.648**	step	-	0.625	7.272	balsamic, must, spice
trans-α-Bergamotene	13474-59-4	-0.185	-0.646**	step	-	0.429	10.38	woody, warm, tea
cis-3-Hexenyl isovalerate	35154-45-1	-0.123	-0.645**	step	-	0.579	9.674	fresh, green, apple, fruity, tropical
Heptanoic acid	111-14-8	0.102	0.621**	null	-	-	-	cheesy, sour, rancid
Hexanoic acid	142-62-1	0.089	0.615**	null	-	-	-	cheesy, fatty
(Z)-β-Ocimene	3338-55-4	-0.149	-0.606**	linear	3.321	-	-	citrus, herbal, floral
(E)-2-Hexenyl acetate	2497-18-9	-0.106	-0.592**	linear	1.676	-	-	sweet, apple skin, banana peel, waxy
1-Nonanol	143-08-8	-0.104	-0.59**	linear	1.716	-	-	fatty, green, orange
Decanal	112-31-2	0.063	0.569*	null	-	-	-	citrus, sweet, waxy
Cyclopentenone	930-30-3	0.091	0.54*	null	-	-	-	-
trans-Linalool oxide (furanoid)	5989-33-3	-0.104	-0.513*	null	-	-	-	earthy, floral, sweet, woody
γ-Nonalactone	104-61-0	-0.122	-0.508*	step	-	0.579	9.411	coconut, creamy, waxy, sweet, buttery
γ-Butyrolactone	96-48-0	0.096	0.507*	step	-	0.625	4.725	caramel, fatty, sweet
2	-	0.1	0.494*	null	-	-	-	-
p-Xylene	106-42-3	-0.115	-0.493*	linear	2.198	-	-	sweet
1-Octen-3-ol	3391-86-4	0.086	0.493*	null	-	-	-	earthy, green, vegetative, mushroom
Benzyl nitrile	140-29-4	-0.066	-0.491*	null	-	-	-	-
Octanoic acid	124-07-2	0.079	0.488*	null	-	-	-	cheesy, fatty, waxy
Butylated hydroxytoluene	128-37-0	-0.091	-0.481*	null	-	-	-	phenolic, camphor
Linalool	78-70-6	-0.114	-0.477*	null	-	-	-	flower, lavender
Cyclopentanone	120-92-3	0.125	0.475*	linear	-2.219	-	-	minty
Coumaran	496-16-2	-0.131	-0.47*	step	-	0.769	9.943	-

*** p < 0.001, ** p < 0.01, * p < 0.05

Table 2. Biomarkers of visible leafhopper damage in order of the strength of correlation to the RDA constrained axis. For each compound, the type of univariate relationship between log transformed relative peak areas percent damage to the focal DCSE leaf is reported. For step function relationships, the change point is reported in units of leafhoppers per young leaf.

Compound	CAS	Multivariate		Univariate				Aroma
		RDA Loading	RDA Correlation	Response type	Linear slope	Change point	ΔIntercept	
1-Hexanol	111-27-3	0.2	0.801***	linear	0.166	-	-	resin, flower, green
(3Z)-Hexenyl hexanoate	31501-11-8	0.175	0.768***	linear	0.15	-	-	green, fruity, fatty, tropical
cis-3-Hexenyl isovalerate	35154-45-1	0.199	0.727***	step	-	8.541	10.545	fresh, green, apple, fruity, tropical
(Z)-2-Hexenol	928-94-9	0.175	0.663**	linear	0.138	-	-	leaf, green, wine, fruit
Coumaran	496-16-2	0.162	0.651**	hinge	0.167 ^a	8.541	-	-
cis-Butyric acid, 3-hexenyl ester	16491-36-4	0.155	0.645**	linear	0.134	-	-	wine, green
γ-Nonalactone	104-61-0	0.145	0.629**	linear	0.089	-	-	coconut, creamy, waxy, sweet, buttery
Benzyl alcohol	100-51-6	0.15	0.625**	step	-	2.4	7.916	fruity, floral, sweet
Methyl salicylate	119-36-8	0.176	0.62**	linear	0.073	-	-	wintergreen
Benzothiazole	95-16-9	0.149	0.617**	linear	0.077	-	-	rubbery, sulfury, vegetal, gasolinear
Phenethyl alcohol	60-12-8	0.172	0.6**	linear	0.147	-	-	honey, spice, rose, lilac
Isopropyl tetradecanoate	110-27-0	0.113	0.594**	linear	0.02	-	-	fatty, oily
(3-hydroxy-2,4,4-trimethylpentyl), 2-methylpropanoate	74367-34-3	0.124	0.59**	null	-	-	-	-
10,18-Bisnorabieta-8,11,13-triene	32624-67-2	0.222	0.584*	linear	0.06	-	-	-
Isovaleric acid	503-74-2	-0.118	-0.564*	step	-	4.206	2.867	sour, cheesy, rancid
cis-Methyl dihydrojasmonate	39647-11-5	-0.185	-0.553*	linear	-0.105	-	-	jasmine, floral, green
N,N-Dibutylformamide	761-65-9	0.106	0.533*	null	-	-	-	-
Diendiol I	13741-21-4	0.144	0.527*	linear	0.116	-	-	-
Benzoic acid	65-85-0	0.06	0.5*	null	-	-	-	balsam, faint, urine
Phenylacetaldehyde	122-78-1	0.125	0.488*	null	-	-	-	floral, honey, sweet
Mesityl oxide	141-79-7	0.06	0.481*	null	-	-	-	acrylic, earthy, sweet, chemical
Ethyl benzoate	93-89-0	0.087	0.48*	null	-	-	-	sweet, wintergreen, fruity, medicinal
o-Hydroxybiphenyl	90-43-7	0.093	0.476*	null	-	-	-	-
Decanoic acid	334-48-5	0.147	0.474*	linear	0.15	-	-	fatty, sour, rancid
cis-Linalool oxide (pyranoid)	14009-71-3	0.109	0.472*	null	-	-	-	citrus, green

*** p < 0.001, ** p < 0.01, * p < 0.05

^aSlope after the change point