RSC Advances

Supplemental material

Antifungal mechanism of cinnamaldehyde and citral combination against *Penicillium expansum* based on FT-IR fingerprint, plasma membrane, oxidative stress and volatile profile

Yuan Wang[1,2,3,4], Kewei Feng[5], Haihua Yang[2,3,4], Yahong Yuan[2,3,4], Tianli Yue[1,2,3,4]*

[1] Northwest University, College of Food Science and Engineering, Xi'an, Shaanxi 710069, China. [2] Northwest A&F University, College of Food Science and Engineering, Yangling, Shaanxi 712100, China. [3] Laboratory of Quality & Safety Risk Assessment for Agro-products (YangLing), Ministry of Agriculture, Yangling, Shaanxi 712100, China. [4] National Engineering Research Center of Agriculture Integration Test (Yangling), Yangling, Shaanxi 712100, China. [5] Northwest A&F University, State Key Laboratory of Crop Stress Biology in Arid Areas, College of Agronomy, Yangling 712100, China.

***Correspondence to: Prof. Dr. Tianli Yue**

College of Food Science and Engineering, Northwest University, Xi'an, Shaanxi 710069, China.
College of Food Science and Engineering, Northwest A&F University, Yangling, Shaanxi, 712100, China.
E-mail address: yuetl305@nwsuaf.edu.cn
Tel: +86-29-87092261
Fax: +86-29-87092261

Table captions

Table S1 MIC, MFC, $MIC_{cin/cit}$ and FICI of cinnamaldehyde and citral against *P. expansum* F-WY-12-02.

Table S2 List of VOCs identified from controls and *P. expansum* F-WY-12-02 grown in PDB supplemented with Cin/Cit.

Table S1 MIC, MFC, $MIC_{cin/cit}$ and FICI of cinnamaldehyde and citral against *P. expansum* F-WY-12-02.

	MIC[a] (mg l^{-1})	MFC[b] (mg l^{-1})	$MIC_{cin/cit}$[c] (mg l^{-1})	FICI[d]
cinnamaldehyde	90	100	45	1
citral	140	150	70	

[a] The minimum inhibitory concentration.

[b] The minimum fungicidal concentration.

[c] The minimum inhibitory concentration of cinnamaldehyde (Cin) and citral (Cit) in their combination (Cin/Cit), respectively.

[d] Fractional Inhibitory Concentration Index. Synergy (FICI ≤ 0.5), addition (0.5 < FICI ≤ 1), indifference (1 < FICI ≤ 4), or antagonism (FIC > 4).

Table S2 List of VOCs identified from controls and *P. expansum* F-WY-12-02 grown in PDB supplemented with Cin/Cit.

	RI	Volatile compound	Contro	Cin/Cit	PDB	PDB/C		RI	Volatile compound	Contro	Cin/Cit	PDB	PDB/C
		Alcohols							**Esters**				
X1	463	Ethanol	X	X	X	X	X79	586	Ethyl Acetate	-	-	X	X
X2	482	Isopropyl Alcohol	X	X	X	X	X80	869	2-Butenoic acid, 3-methyl-, ethyl ester	-	X	-	-
X3	562	1-Propanol	X	-	-	-	X81	869	Ethyl tiglate	X	-	-	-
X4	597	1-Propanol, 2-methyl-	X	-	-	-	X82	992	2-Hexenoic acid, ethyl ester	-	X	-	-
X5	697	1-Butanol, 3-methyl-	X	X	-	-	X83	1180	Formic acid, octyl ester	X	-	X	-
X6	697	1-Butanol, 2-methyl-	X	X	-	-	X84	1183	Octanoic acid, ethyl ester	X	-	-	-
X7	728	3-Buten-1-ol, 3-methyl-	X	X	-	-	X85	1215	Oxiranecarboxaldehyde, 3-methyl-3-(4-methyl-3-pentenyl)-	-	X	-	-
X8	743	2,3-Butanediol	X	-	-	-	X86	1284	2-Propenoic acid, 2-methyl-, 1,2-ethanediyl ester	X	X	-	-
X9	845	3-Penten-1-ol, 4-methyl-	-	X	-	-	X87	1380	Propanoic acid, 2-methyl-, 3-hydroxy-2,2,4-trimethylpentyl ester	X	-	X	-
X10	964	5-Hepten-2-ol, 6-methyl-	-	X	-	-	X88	1520	Glutaric acid, di(isobutyl) ester	X	X	-	-
X11	969	1-Octen-3-ol	-	X	-	-	X89	1557	2-Butenedioic acid (Z)-, dibutyl ester	X	-	-	-
X12	985	6-Hepten-1-ol, 2-methyl-	-	X	-	-	X90	1605	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	X	X	X	X
X13	995	2-Propyl-1-pentanol	X	-	-	-	X91	1619	Hexanedioic acid, bis(2-methylpropyl) ester	X	X	-	-
X14	995	1-Hexanol, 2-ethyl-	-	-	X	-	X92	1653	Tributyl phosphate	X	X	-	-
X15	1059	Eucalyptol	X	-	-	-	X93	1878	Hexadecanoic acid, methyl ester	-	X	-	-
X16	1059	1-Octanol	X	X	-	-	X94	1882	Oxalic acid, 2-ethylhexyl hexyl ester	X	-	-	-
X17	1072	1,5,7-Octatrien-3-ol, 3,7-dimethyl-	-	X	-	-	X95	1908	1,2-Benzenedicarboxylic acid,bis(2-methylpropyl) ester	X	X	X	-

X18	1082	Linalool	X	X	-	-	X96	1978	Hexadecanoic acid, ethyl ester	X	-	-	-
X19	1136	Phenylethyl Alcohol	X	X	-	-	X97	2037	Dibutyl phthalate	X	X	-	-
X20	1137	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)-	-	X	-	-	X98	2276	Nonadecanoic acid, ethyl ester	X	-	-	-
X21	1143	L-.alpha.-Terpineol	X	X	-	-			**Ketones**				
X22	1146	4-Hexen-1-ol,5-methyl-2-(1-methylethenyl)-, (R)-	-	X	-	-	X99	455	Acetone	X	-	-	-
X23	1159	1-Nonanol	X	-	-	-	X100	820	5-Hexen-2-one, 5-methyl-	X	-	-	-
X24	1164	cis-Linalool oxide	-	X	-	-	X101	853	2-Heptanone	X	-	X	-
X25	1164	Cyclohexanol,5-methyl-2-(1-methylethyl)-, (1α,2β,5α)-	X	-	-	-	X102	938	5-Hepten-2-one, 6-methyl-	-	X	-	-
X26	1179	6-Octen-1-ol, 3,7-dimethyl-, (R)-	-	X	-	-	X103	952	3-Octanone	X	-	X	-
X27	1228	2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-	-	X	-	-	X104	1029	Acetophenone	-	-	X	-
X28	1228	2,6-Octadien-1-ol, 3,7-dimethyl-, (E)-	-	X	-	-	X105	1121	(+)-2-Bornanone	X	-	-	-
X29	1230	2-Cyclohexene-1-methanol, 2,6,6-trimethyl-	-	X	-	-	X106	1158	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)-	-	X	-	-
X30	1243	2-Propen-1-ol, 3-phenyl-	-	X	-	-	X107	1190	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethenyl)-, (S)-	-	X	-	-
X31	1258	1-Decanol	X	-	-	-	X108	1420	5,9-Undecadien-2-one, 6,10-dimethyl-	-	-	X	-
X32	1357	1-Undecanol	X	-	-	-			**Phenols**				
X33	1457	1-Dodecanol	X	-	-	-	X109	983	Benzene, 1-methoxy-3-methyl-	X	-	-	-
X34	1543	Cedrol	X	X	-	-	X110	1014	Phenol, 3-methyl-	X	X	-	-
		Aldehydes					X111	1077	Benzene, (2-methyl-1-propenyl)-	-	X	-	X
X35	408	Acetaldehyde	X	X	-	-	X112	1235	1,4-Benzenediol, 2-methyl-	-	X	-	-
X36	543	Propanal, 2-methyl-	X	-	-	-	X113	1261	Benzene, 4-ethenyl-1,2-dimethoxy-	X	-	-	-
X37	643	Butanal, 3-methyl-	X	-	-	-	X114	1271	Benzene, 4-ethyl-1,2-dimethoxy-	X	-	-	-

X38	806	Hexanal	X	X	X	-	X115	1480	1,1'-Biphenyl, 2-methyl-	-	-	X	-
X39	905	Heptanal	X	X	X	-	X116	1555	Phenol, 2,5-bis(1,1-dimethylethyl)-	X	X	X	X
X40	982	Benzaldehyde	X	X	X	X	X117	1566	Diphenylamine	X	X	-	-
X41	1005	Octanal	X	X	-	-	X118	1633	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	-	-	X	-
X42	1013	2-Octenal, (E)-	-	-	X	-	X119	1668	Butylated Hydroxytoluene	-	X	-	-
X43	1081	Benzeneacetaldehyde	X	-	X	-	X120	1902	Phenol, 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-	-	-	X	-
X44	1095	Benzaldehyde, 3-methyl-	-	-	X	-	X121	1950	2,6-Di-tert-butyl-4-nitrophenol	X	-	-	-
X45	1095	Benzaldehyde, 2-methyl-	-	-	X	-			**Terpenes**				
X46	1104	Nonanal	X	X	X	-	X122	897	Sabinene	-	X	-	-
X47	1112	2-Nonenal, (E)-	-	-	X	-	X123	958	β-Myrcene	-	X	-	-
X48	1125	6-Octenal, 3,7-dimethyl-, (R)-	-	X	-	-	X124	976	1,3,6-Octatriene, 3,7-dimethyl-, (Z)-	-	X	-	-
X49	1186	1,3-Cyclohexadiene-1-carboxaldehyde, 2,6,6-trimethyl-	-	X	-	-	X125	998	γ-Terpinene	-	X	-	-
X50	1189	Cinnamaldehyde, (E)-	-	X	-	X	X126	1018	D-Limonene	-	X	-	-
X51	1204	Decanal	-	X	-	-	X127	1052	α-Terpinolene	-	X	-	-
X52	1212	2-Decenal, (E)-	-	-	X	-	X128	1125	Isoneroloxide	-	X	-	-
X53	1402	Dodecanal	X	-	-	-	X129	1147	6-Octenal, 7-methyl-3-methylene-	-	-	-	X
X54	1601	Tetradecanal	X	-	-	-	X130	1174	2,6-Octadienal, 3,7-dimethyl-, (E)-	-	X	-	X
X55	1701	Pentadecanal	X	-	-	-	X131	1174	2,6-Octadienal, 3,7-dimethyl-, (Z)-	-	X	-	X
X56	1856	3,5-di-tert-Butyl-4-hydroxybenzaldehyde	X	X	-	-	X132	1174	Citral	-	-	-	X
		Alkanes					X133	1175	1-p-Menthen-9-al	-	X	-	-
X57	518	Pentane	X	X	-	-	X134	1184	3,6-Octadienal, 3,7-dimethyl-, (E)-	-	-	-	X
X58	788	Heptane, 2,3-dimethyl-	X	-	-	-			**Acids**				

X59	1165	Decane, 2,8,8-trimethyl-	-	-	X	-	X135	1272	Nonanoic acid	X	-	-	-
X60	1185	Nonane, 3-methyl-5-propyl-	-	-	X	-	X136	1293	(R)-(+)-Citronellic acid；	-	X	-	-
X61	1320	Dodecane, 2,6,10-trimethyl-	X	-	-	-	X137	1375	2,6-Octadienoic acid, 3,7-dimethyl-, (E)-	-	-	-	X
X62	1413	Tetradecane	X	-	X	-	X138	1461	9-Oxononanoic acid	X	-	-	-
X63	1448	Tetradecane, 4-methyl-	X	-	-	-	X139	1968	n-Hexadecanoic acid	X	-	-	
X64	1465	2,6,10-Trimethyltridecane	X	-	X	-			**Other categery**				
X65	1555	Cyclopentane, decyl-	X	-	-	-	X140	722	Disulfide, dimethyl	X	-	-	-
X66	1576	n-Nonylcyclohexane	X	-	X	-	X141	972	Dimethyl trisulfide	X	-	-	-
X67	1627	5,5-Dibutylnonane	X	-	X	-	X142	1111	cis-Rose oxide	-	X	-	-
X68	1653	Pentadecane, 2,6,10,14-tetramethyl-	X	-	X	-	X143	1208	Benzothiazole	X	-	X	-
X69	1711	Heptadecane	X	X	X	X	X144	1301	Oxime-, methoxy-phenyl-_	X	X	X	-
X70	1753	Hexadecane, 2,6,11,15-tetramethyl-	-	-	X	-	X145	1548	2-(Methylmercapto)benzothiazole	-	X	-	X
X71	1753	Hexadecane, 2,6,10,14-tetramethyl-	-	-	X	-							
X72	2009	Eicosane	X	X	X	-							
X73	2036	Octadecane, 1-chloro-	X	-	-	-							
X74	2109	Heneicosane	X	-	X	-							
X75	2332	11-Methyltricosane	X	-	-	X							
X76	2664	2-Methylhexacosane	X	-	-	-							
X77	2840	2-methyloctacosane	-	X	-	-							
X78	3997	Tetracontane	X	-	-	-							

X: Detected; -: Undetected.

Control: *P. expansum* grown in PDB (positive control).

Cin/Cit: *P. expansum* grown in PDB/Cin/Cit (treatment group).

PDB: PDB medium alone (negative control-1).

PDB/C: PDB/Cin/Cit without fungal inoculation (negative control-2).