Supplementary materials

Endophytic bacterium-triggered reactive oxygen species directly increasing oxygenous sesquiterpenoid content and diversity in *Atractylodes lancea*

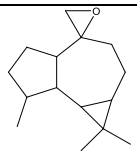
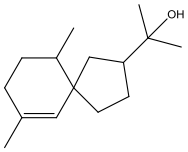
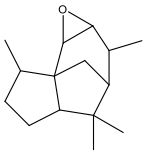
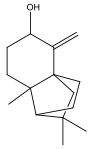
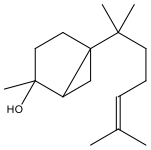
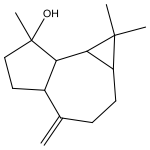
RUNNING TITLE ROS directly impact plant sesquiterpenoid compositions

Jia-Yu Zhou,[a] Jie Yuan,[a] Xia Li,[b] Yi-Fan Ning,[a] Chuan-Chao Dai[a#]

Jiangsu Key Laboratory for Microbes and Functional Genomics, Jiangsu Engineering and Technology Research Center for Industrialization of Microbial Resources, College of Life Sciences, Nanjing Normal University, Nanjing, Jiangsu Province, China[a]; Jiangsu High Quality Rice Research and Development Center, Nanjing Branch of China National Center Rice Improvement, Institute of Food Crops, Jiangsu Academy of Agricultural Sciences, Nanjing, Jiangsu Province, China[b]

[#] Corresponding author, e-mail: daichuanchao@njnu.edu.cn

TABLE S1 Oxygenous sesquiterpenoids derived from *in vitro* oxidation by singlet oxygen

Peak order	Retention time (min)	Compound	Molecular weight	Chemical formula	Chemical structure formula
1	17.764	Aromadendrene oxide	220.35	$C_{15}H_{24}O$	
2	18.125	Hinesol	222.37	$C_{15}H_{26}O$	
3	19.234	Diepicedrene-1-oxide	220.35	$C_{15}H_{24}O$	
4	19.388	Tricyclo[5.2.2.0(1,6)]undecan-3-ol, 2-methylene-6,8,8-trimethyl-	220.35	$C_{15}H_{24}O$	
5	19.548	7-epi-cis-Sesquisabinene hydrate	222.37	$C_{15}H_{26}O$	
6	20.852	Spathulenol	220.35	$C_{15}H_{24}O$	

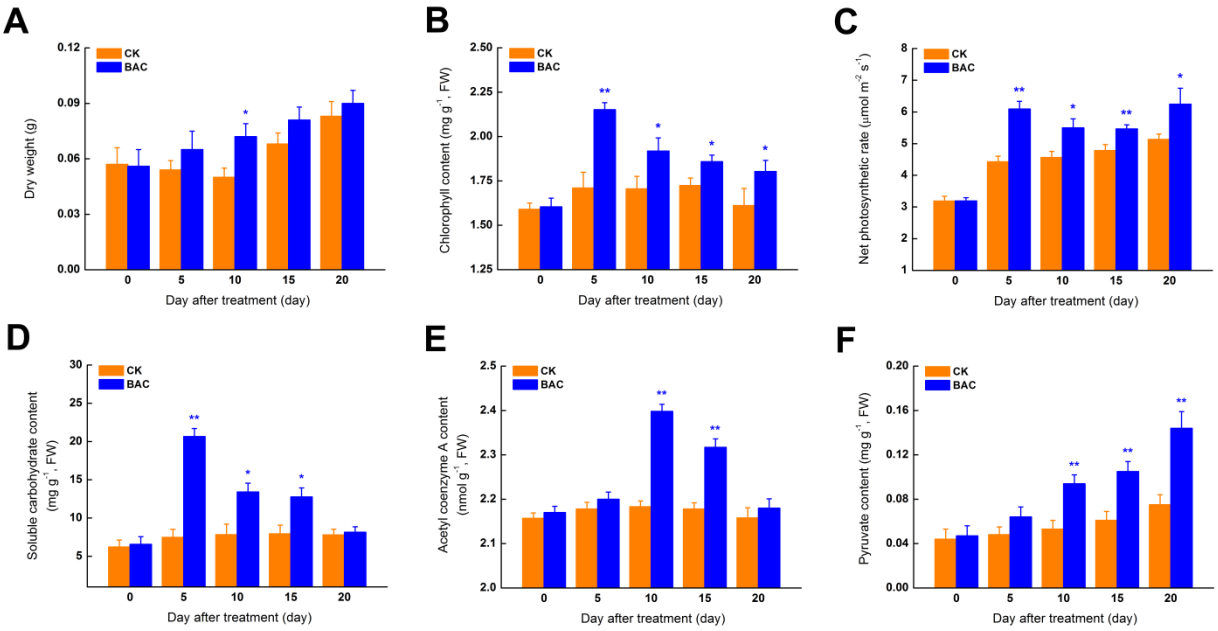


FIG S1 Impacts of *Pseudomonas fluorescens* ALEB7B colonization on *Atractylodes lancea* primary metabolism over time. (A) Plant dry weight. (B) Leaf chlorophyll content. (C) Leaf net photosynthetic rate. (D) Plant soluble carbohydrate content. (E) Plant acetyl coenzyme A content. (F) Plant pyruvate content. Results are means for three biological replicates. Error bars indicate standard deviations. * indicates significant differences at $P < 0.05$ and ** indicates significant differences at $P < 0.01$. CK stands for control. BAC stands for *P. fluorescens* ALEB7B.

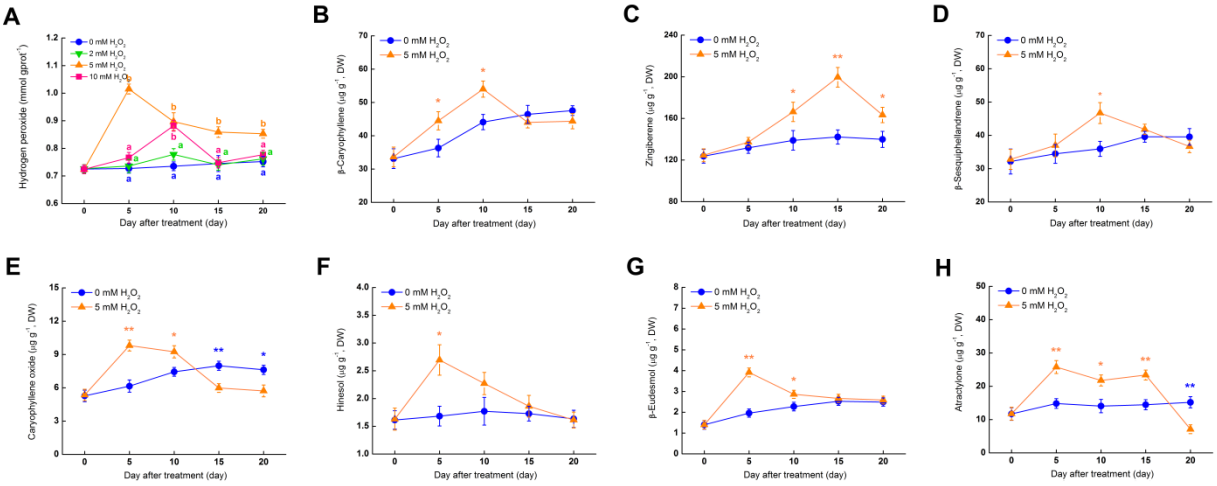


FIG S2 Content of endogenous hydrogen peroxide and seven main sesquiterpenoids in *Atractylodes lancea* treated with exogenous hydrogen peroxide over time. (A) Hydrogen peroxide. (B) β-Caryophyllene. (C) Zingiberene. (D) β-Sesquiphellandrene. (E) Caryophyllene oxide. (F) Hinesol. (G) β-Eudesmol. (H) Atractylone. Results are means for three biological replicates. Error bars indicate standard deviations. Different lowercase letters indicate significant differences at $P < 0.05$. * indicates significant differences at $P < 0.05$ and ** indicates significant differences at $P < 0.01$. H_2O_2 stands for hydrogen peroxide.

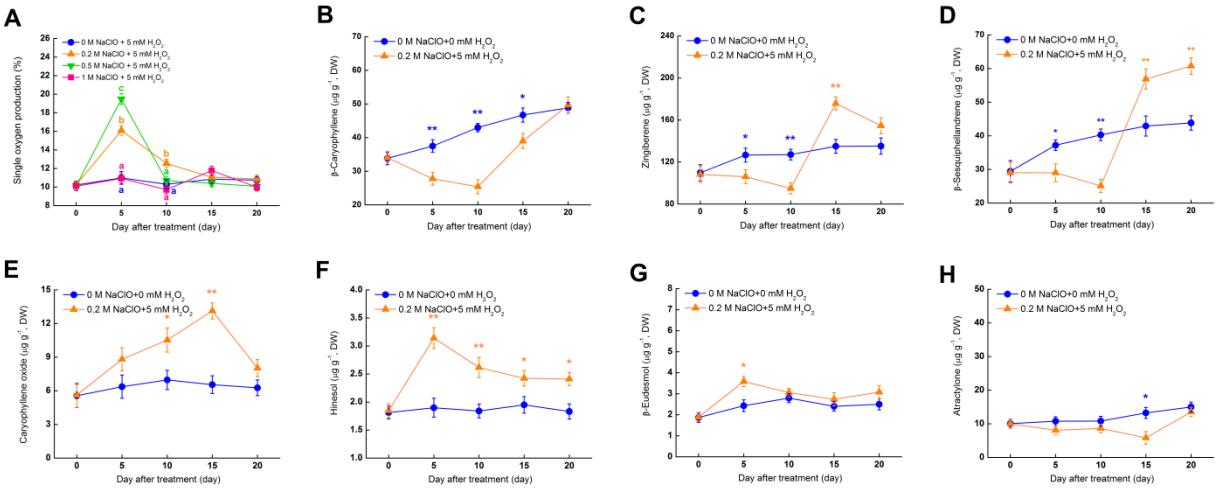


FIG S3 Content of endogenous single oxygen and seven main sesquiterpenoids in *Atractylodes lancea* treated with exogenous sodium hypochlorite and hydrogen peroxide over time. (A) Single oxygen. (B) β-Caryophyllene. (C) Zingiberene. (D) β-Sesquiphellandrene. (E) Caryophyllene oxide. (F) Hinesol. (G) β-Eudesmol. (H) Atractylone. Results are means for three biological replicates. Error bars indicate standard deviations. Different lowercase letters indicate significant differences at $P < 0.05$. * indicates significant differences at $P < 0.05$ and ** indicates significant differences at $P < 0.01$. NaClO stands for sodium hypochlorite. H_2O_2 stands for hydrogen peroxide.

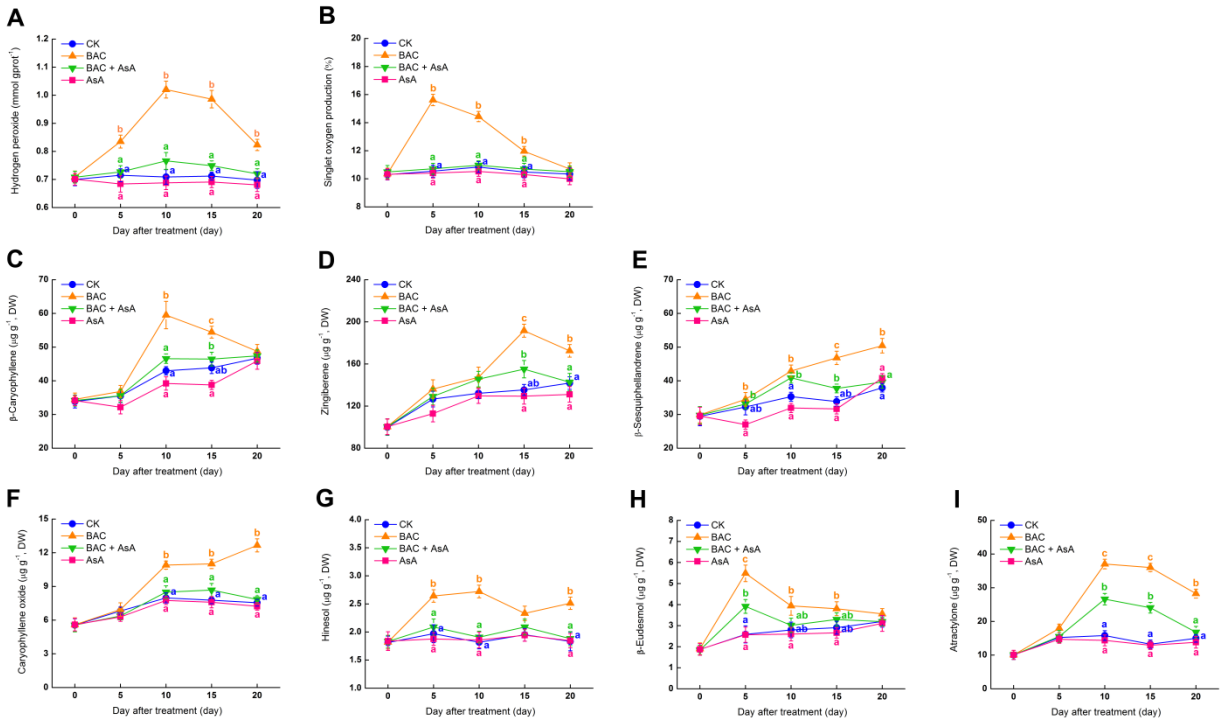


FIG S4 Content of endogenous hydrogen peroxide, single oxygen, and seven main sesquiterpenoids in *Atractylodes lancea* treated with ascorbic acid before bacterial inoculation over time. (A) Hydrogen peroxide. (B) Single oxygen. (C) β-Caryophyllene. (D) Zingiberene. (E) β-Sesquiphellandrene. (F) Caryophyllene oxide. (G) Hinesol. (H) β-Eudesmol. (I) Atractylone. Results are means for three biological replicates. Error bars indicate standard deviations. Different lowercase letters indicate significant differences at $P < 0.05$. * indicates significant differences at $P < 0.05$ and ** indicates significant differences at $P < 0.01$. CK stands for control. BAC stands for *P. fluorescens* ALEB7B. AsA stands for ascorbic acid.

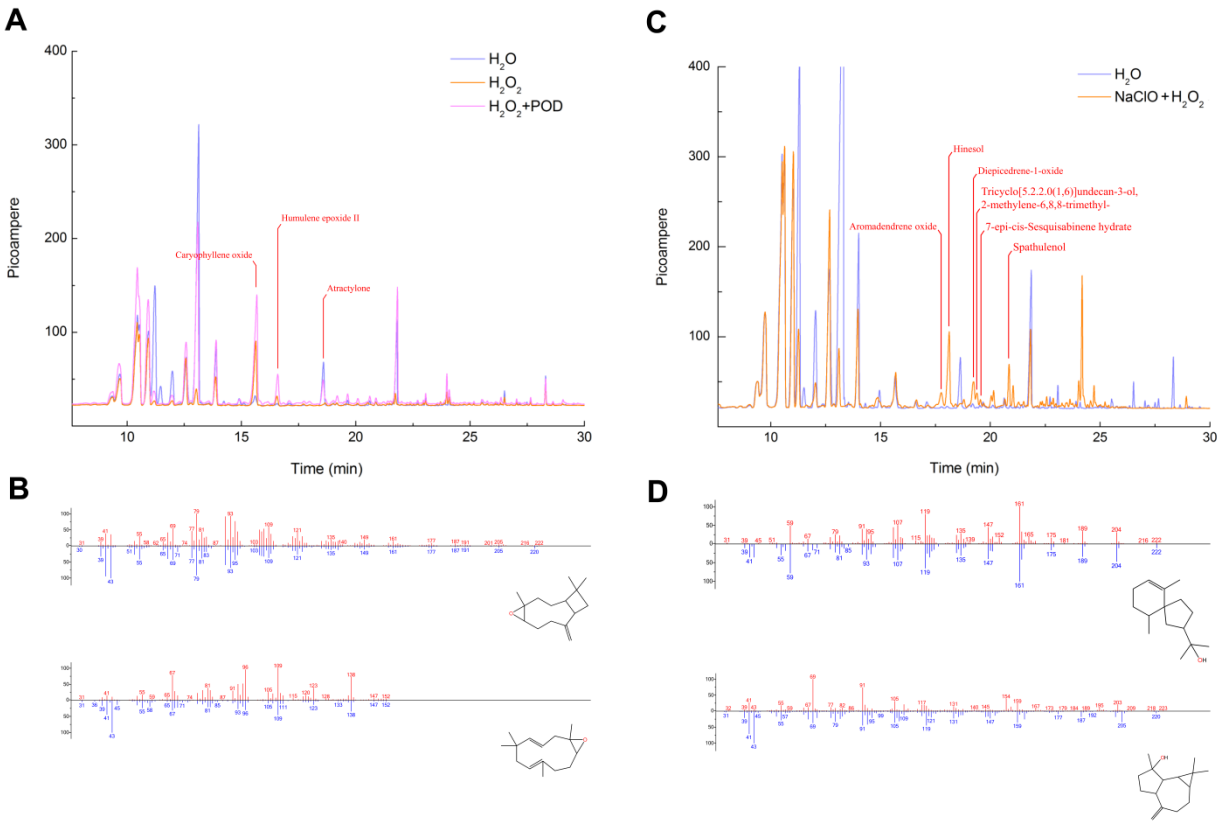


FIG S5 Total ion chromatogram and mass spectrogram of oxidized products in total extracted sesquiterpenoids treated with oxidants. (A) Total ion chromatogram of oxidized products in total extracted sesquiterpenoids treated with hydrogen peroxide and hydrogen peroxide + peroxidase. (B) Mass spectrogram of caryophyllene oxide and humulene epoxide II. (C) Total ion chromatogram of oxidized products in total extracted sesquiterpenoids treated with hydrogen peroxide + sodium hypochlorite. (D) Mass spectrogram of hinesol and spathulenol. H_2O_2 stands for hydrogen peroxide. POD stands for peroxidase. NaClO stands for sodium hypochlorite.