

Early Detection of Sage (*Salvia officinalis* L.) Responses to Ozone Using Reflectance Spectroscopy

Table S1. Summary of measurement design showing plants measured (*) at 0, 1, 2, 5, 8, and 24 h from the beginning of the exposure for analyses of spectral signatures (SS) and for PLSR-modelling (PLSR). Treatments (Treatm; control (C) versus ozone (O₃)) and numbers of exposure chambers are also specified.

Plant	Treatm	Chamb	0 h		1 h		2 h		5 h		8 h		24 h	
			SS	PLSR	SS	PLSR	SS	PLSR	SS	PLSR	SS	PLSR	SS	PLSR
1	C	1	*		*		*		*		*		*	
2	C	1		*		*		*		*				
3	C	1				*		*		*		*		
4	C	1	*		*		*		*		*		*	*
5	C	1							*		*			
6	C	1					*		*		*			
7	C	1									*		*	
8	C	1	*		*		*		*		*		*	*
9	C	2					*		*		*			
10	C	2	*		*		*		*		*		*	*
11	C	2		*		*		*		*				
12	C	2				*		*		*		*		
13	C	2							*		*			
14	C	2		*		*		*		*				
15	C	2	*		*		*		*		*		*	*
16	C	2									*		*	
17	C	2		*		*		*		*				
18	C	2	*		*		*		*		*			
19	O ₃	3					*		*		*			
20	O ₃	3	*		*		*		*		*		*	
21	O ₃	3			*		*		*		*			
22	O ₃	3				*		*		*		*		
23	O ₃	3	*		*		*		*		*		*	*
24	O ₃	3			*		*		*		*	*		*
25	O ₃	3				*		*		*		*		
26	O ₃	3	*		*		*		*		*		*	*
27	O ₃	3							*		*			
28	O ₃	4					*		*		*			
29	O ₃	4	*		*		*		*		*		*	*
30	O ₃	4			*		*		*		*	*		*
31	O ₃	4				*		*		*		*		
32	O ₃	4	*		*		*		*		*		*	*
33	O ₃	4			*		*		*		*	*		*
34	O ₃	4					*		*		*			
35	O ₃	4	*		*		*		*		*		*	*
36	O ₃	4							*		*			
Tot C plants			6	4	6	6	6	8	6	10	6	8	6	7
Tot O ₃ plants			6	0	10	3	10	6	10	9	9	12	6	8

Table S2. Tested ranges of (i) preliminary PLSR-models used the estimation of leaf traits by spectral data, and (ii) preliminary PERMANOVA for the effects of ozone, time, and their interaction on reflectance profiles of sage leaves. Final ranges are in bold. Trait abbreviations: A, CO₂ assimilation rate; E, transpiration; g_s, stomatal conductance; C_i, intercellular CO₂ concentration; WUE_i, instantaneous water use efficiency; WUE_{in}, intrinsic water use efficiency; *k*, instantaneous carboxylation efficiency; T_l, temperature of adaxial leaf surface; MDA, malondialdehyde; ORAC, oxygen radical absorption capacity; HORAC, hydroxyl radical antioxidant capacity; DHA, oxidized ascorbate; DHA/ASA_{TOT}, oxidized:total ascorbate ratio; GSH, reduced glutathione; GSH_{TOT}, total glutathione; Chl *a*, chlorophyll *a*; Chl_{TOT}, total chlorophyll; Car, carotenoids; Phen, total phenols.

Trait	Tested Ranges (nm)
A	400–2400, 950–2400, 1400–2400, 400–900, 600–900, 500–1100, 400–1200, 400–1100, 400–1000
E	400–2400 , 400–1200, 950–2400, 1100–2400, 1400–2400, 600–900, 500–1100
g _s	400–2400, 400–1200, 1400–2400, 950–2400
C _i	400–2400, 400–1200, 1400–2400, 950–2400
WUE _i	400–2400 , 950–2400, 1400–2400, 400–1200
WUE _{in}	400–2400 , 400–1200, 500–1100, 600–900, 900–1200
<i>k</i>	400–2400, 950–2400, 1400–2400, 400–1200, 600–900, 500–1100, 400–1100, 400–1000
T _l	400–2400 , 950–2400, 1400–2400, 400–900, 600–900
MDA	400–2400, 950–2400, 1100–2400, 1400–2400, 500–1100, 400–1200, 400–750 + 1100–2400, 400–750 + 1400–2400
ORAC	400–2400, 950–2400, 1100–2400, 950–1800, 1200–1800, 950–1600, 1400–1800, 1800–2250, 1400–2400
HORAC	400–2400, 950–2400, 1100–2400, 950–1800, 1200–1800, 950–1600, 1400–1800, 1800–2250, 1400–2400
DHA	400–2400, 950–2400, 1100–2400, 500–1100, 600–900, 950–2250, 950–1800, 1100–1400 + 1600–1800, 1100–1400 + 1800–2250, 1100–1800
DHA/ASA _{TOT}	400–2400, 500–1100, 600–900, 950–2400, 1400–2400, 1100–2400, 1100–1800
GSH	400–2400, 950–2400, 1400–2400, 400–1200, 500–1100, 600–900, 400–750, 400–900
GSH _{TOT}	400–2400 , 950–2400, 1400–2400, 400–1200, 400–900, 600–900, 500–1100, 400–1800, 900–1200, 1100–2400, 400–700 + 950–2400, 400–700 + 950–1400, 400–1100 + 1800–2400, 400–750 + 1400–2400
Chl <i>a</i>	400–2400, 400–1800, 400–1200, 400–900, 600–900, 500–1100, 400–800, 400–700, 400–700 + 900–1200, 400–700 + 1400–1800, 400–700 + 1600–1800
Chl _{TOT}	400–2400 , 400–1800, 400–1200, 500–1100, 400–1000, 400–900, 400–800, 600–900, 950–2400, 400–700 + 1100–1800, 400–700 + 950–1800, 400–700 + 1100–2400, 400–700 + 1000–2400, 400–700 + 900–2400, 400–700 + 1400–2400, 400–900 + 1600–2400, 400–900 + 1800–2400, 400–900 + 1200–2400, 400–700 + 1000–2400
Car	400–2400, 400–1200, 500–1100, 600–900, 400–900, 400–700, 400–700 + 1100–1400, 400–600 + 700–800, 950–2400, 950–2250, 950–1400, 1100–1600, 1100–1500, 1200–1800, 1200–1600, 1200–1400, 1000–1400, 1000–1300, 1100–1400
Phen	400–2400, 950–2400, 1100–2400, 1200–2400, 1400–2400, 1600–2400, 1800–2400, 950–1800, 950–1600, 1100–1400, 400–750 + 1400–2400, 1200–1600, 1000–1600, 1100–1500, 1100–1600
PERMANOVA	400–2400 , 400–750, 950–2400, 1400–2400, 2000–2400, 400–1200, 400–1800, 950–1600, 1200–1800, 1400–1800, 400–1400 + 1800–2250, 400–750 + 1200–1600, 400–750 + 950–1200, 400–750 + 1000–2400