

Supplementary Material

# Leaf-scale Study of Biogenic Volatile Organic Compound Emissions from Willow (*Salix* spp.) Short Rotation Coppices Covering Two Growing Seasons

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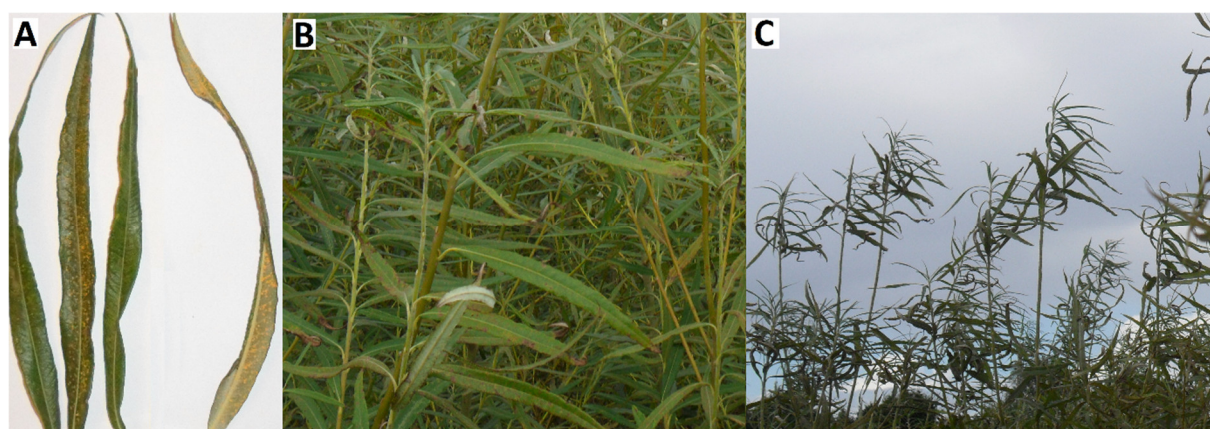
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**Figure S1.** The two plots where the measurements were performed. (A) P1 (58°16'55" N 12°46'20" E) and (B) P2 (58°17'09" N 12°45'31" E). Black marks are the locations of the measurements. Maps are taken and modified from Karlsson et al. (2020) [42].



**Figure S2.** Impact of rust (*Melampsora* spp.) infestation on P1. (A) Visible yellow dots in late July. (B) Lower part of the trees in September where some parts of leaves have changed the color to red/brown (necrotic lesions) and started to fold. (C) Top of the trees in September. Many leaves were shed or folded.



**Figure S3.** (A) Leaves from the higher part (z<sub>H</sub>) of the canopy that were measured with the branch chamber in October showing damage from leaf beetles (*Phratora vulgatissima*). (B) Leaves from the lower part (z<sub>M</sub>) of the canopy in October measured with the branch chamber.

**Table S1.** Pure injected standards in the GC-MS analysis. Numbers in the parentheses are CAS-number.

Hemiterpenes	Monoterpenes	Sesquiterpenes	other VOCs
isoprene * (78-79-5)	α-pinene § (80-56-8)	aromadendrene * (109119-91-7)	2-methylfuran * (534-22-5)
	camphene * (79-92-5)	humulene * (6753-98-6)	toluene § (108-88-3)
	β-pinene § (127-91-3)	nerolidol § (142-50-7)	1-octene § (111-66-0)
	myrcene § (123-35-3)		hexanal * (66-25-1)
	α-phellandrene § (99-83-2)		furfural * (98-01-1)
	p-cymene (99-87-6)		2-hexenal * (505-57-7)
	eucalyptol § (470-82-6)		p-xylene § (106-42-3)
	γ-terpinene § (99-85-4)		o-xylene § (95-47-6)
	ocimene § (502-99-8)		benzaldehyde § (100-52-7)
	terpinolene * (586-62-9)		1-octen-3-ol § (3391-86-4)
	linalool § (78-70-6)		octanal * (124-13-0)
			cis-3-hexenyl acetate § (3681-71-8)
			nonanal § (124-19-6)
			cis-3-hexenyl butyrate § (16491-36-4)

\* These standards were produced by Sigma-Aldrich. § These standards were produced by Supelco.

**Table S2.** Measured (E) and standardized (Es) emission rates ( $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1}$ , n = 663) for all compounds and all measurements. Numbers in parentheses are standard deviation (SD,  $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1}$ ). No standardization is made for OVOCs (-).

BVOC	E ( $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1}$ )	Es ( $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1}$ )
isoprene	23.5 (28.1)	45.2 (42.9)
Tot MTs	0.163 (0.117)	0.301 (0.201)
ocimene	0.137 (0.321)	0.255 (0.540)
limonene *	0.008 (0.042)	0.014 (0.081)
p-cymene	0.006 (0.042)	0.011 (0.069)
linalool	0.006 (0.017)	0.010 (0.035)
α-pinene	0.003 (0.021)	0.005 (0.034)
3-carene *	0.002 (0.019)	0.004 (0.040)
eucalyptol	0.001 (0.010)	0.002 (0.024)



myrcene	<0.001 (<0.001)	<0.001 (<0.001)
allo-ocimene *	<0.001 (<0.001)	<0.001 (<0.001)
Tot SQTs	0.035 (0.062)	0.103 (0.249)
caryophellene +	0.011 (0.031)	0.024 (0.080)
humulene	0.010 (0.090)	0.040 (0.409)
$\alpha$ -farnesene +	0.009 (0.062)	0.017 (0.125)
nerolidol	0.004 (0.049)	0.022 (0.243)
Tot other VOCs	0.751 (0.159)	-
cyclopentyl acetylene §	0.083 (0.205)	-
benzaldehyde (benzenoid)	0.065 (0.163)	-
hexanal (aldehyde)	0.064 (0.320)	-
nonanal (aldehyde)	0.061 (0.147)	-
2-ethylhexanoic acid § (carboxylic acid)	0.059 (0.252)	-
pentanal § (aldehyde)	0.037 (0.226)	-
decanal § (aldehyde)	0.036 (0.148)	-
octanal (aldehyde)	0.030 (0.105)	-
2-methylbutane § (alkane)	0.027 (0.105)	-
2-pentanone § (ketone)	0.026 (0.208)	-
2-ethylhexanol § (alcohol)	0.024 (0.082)	-
2-hexanone § (ketone)	0.023 (0.146)	-
benzoic acid § (carboxylic acid)	0.023 (0.116)	-
1-dodecene § (alkene)	0.022 (0.205)	-
unknown 1 §	0.021 (0.150)	-
pentadecane § (alkane)	0.020 (0.078)	-
heptanal § (aldehyde)	0.019 (0.083)	-
furfural (aldehyde)	0.018 (0.149)	-
toluene (benzenoid)	0.018 (0.051)	-
phenol § (phenol)	0.016 (0.098)	-
cyclopropane, ethylidene- # (hemiterpene)	0.013 (0.033)	-
acetophenone § (ketone)	0.012 (0.049)	-
unknown 2 §	0.012 (0.234)	-
3-methylhexane § (alkane)	0.011 (0.081)	-
tetradecane § (alkane)	0.011 (0.074)	-

\* These MTs were quantified with  $\alpha$ -pinene as injected standard in GC-MS.

+ These SQTs were quantified with humulene as injected standard in GC-MS.

§ These other VOCs were quantified with toluene as injected standard in GC-MS.

# This compound was quantified with isoprene as injected standard in GC-MS.

**Table S3.** Emission rates (STD for isoprene, MTs and SQTs,  $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1}$ ) and fraction (%) of the total BVOC emission or within the BVOC group (MTs and SQTs) from ZH in 2015.

2015 ZH	July	Aug	Sep
isoprene	74.8 (98.5%)	70.4 (97.3%)	19.2 (96.7%)
MTs (tot)	0.580 (0.8%)	0.268 (0.4%)	0.286 (1.4%)
$\alpha$ -pinene	0.036 (6.2 %)	0.007 (2.6%)	0
ocimene	0.540 (93.1 %)	0.256 (95.6%)	0.286 (100%)
linalool	0	0.004 (1.6%)	0
eucalyptol	0.004 (0.7 %)	0.001 (0.2%)	0
SQTs (tot)	0.076 (0.1%)	0.040 (<0.1%)	0.171 (0.9%)



$\alpha$ -farnesene	0.022 (29.3%)	0.014 (35.0%)	0
humulene	<0.001 (0.2%)	0.001 (2.5%)	0
caryophyllene	0.053 (70.5%)	0.025 (62.5%)	0.171 (100%)
OVOCs (tot)	0.441 (0.6%)	1.640 (2.3%)	0.207 (1.0%)
BVOCs (tot)	75.896 (100%)	72.348 (100 %)	19.864 (100%)
T <sub>c</sub>	23.2 (4.7)	28.9 (2.9)	19.3 (3.4)
PAR <sub>c</sub>	562 (397)	467 (230)	329 (192)

Bottom: average T<sub>c</sub> (°C, mean and SD) and PAR<sub>c</sub> ( $\mu\text{mol m}^{-2} \text{s}^{-1}$ , mean and SD) for each month.

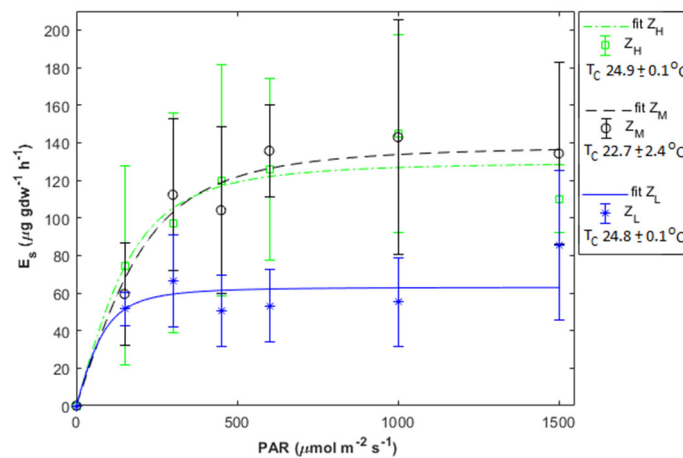
**Table S4.** Values used for the fitted curves in Figure 3. E<sub>s</sub> is the emission factor ( $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1}$ ), C<sub>L</sub> is the correction factor for light (calculated by using mean PAR<sub>c</sub> for the whole season and year, and  $\alpha$ , T<sub>s</sub> and C<sub>L1</sub> adopted from Guenther et al. (1993) [55]). C<sub>T1</sub> (J mol<sup>-1</sup>), C<sub>T2</sub> (J mol<sup>-1</sup>) and T<sub>m</sub> (K) are empirical constants.

	2015	2016
E <sub>s</sub> ( $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1}$ )	93.8	97.1
C <sub>L</sub>	0.8317	0.8688
C <sub>T1</sub>	148700	135300
C <sub>T2</sub>	211000	103000
T <sub>m</sub> (K)	307	298

**Table S5.** Slope (E/PAR,  $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1} \mu\text{mol}^{-1} \text{m}^2 \text{s}$ , n = 3–6) between different PAR values at different height levels for the fitted curves in Figure 4A.

PAR	Lower (z <sub>L</sub> )	Middle (z <sub>M</sub> )	Higher (z <sub>H</sub> )
0–150 $\mu\text{mol m}^{-2} \text{s}^{-1}$	0.058	0.112	0.140
150–300 $\mu\text{mol m}^{-2} \text{s}^{-1}$	0.051	0.093	0.111
300–450 $\mu\text{mol m}^{-2} \text{s}^{-1}$	0.042	0.067	0.075
450–600 $\mu\text{mol m}^{-2} \text{s}^{-1}$	0.033	0.045	0.048
600–1000 $\mu\text{mol m}^{-2} \text{s}^{-1}$	0.020	0.023	0.023
1000–1500 $\mu\text{mol m}^{-2} \text{s}^{-1}$	0.009	0.008	0.008
E <sub>s</sub> ( $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1}$ )	30.7	147.9	242.1
C <sub>T</sub>	0.5142	0.3880	0.5207
$\alpha$	0.0013	0.0018	0.002
C <sub>L1</sub>	2.83	1.13	0.58

Bottom: values for the fitted parameters in Figure 4A.



**Figure S4.** Standardized isoprene emissions rates ( $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1}$ , mean  $\pm$  SD,  $n = 3\text{--}6$ ) and fitted curves for different PAR values ( $\mu\text{mol m}^{-2} \text{s}^{-1}$ ) using Equation (7) below at different heights. Values for the parameters can be seen in Table S10 below.

$$E_S = E_S^p \times C_T \times C_L \quad (\text{S1})$$

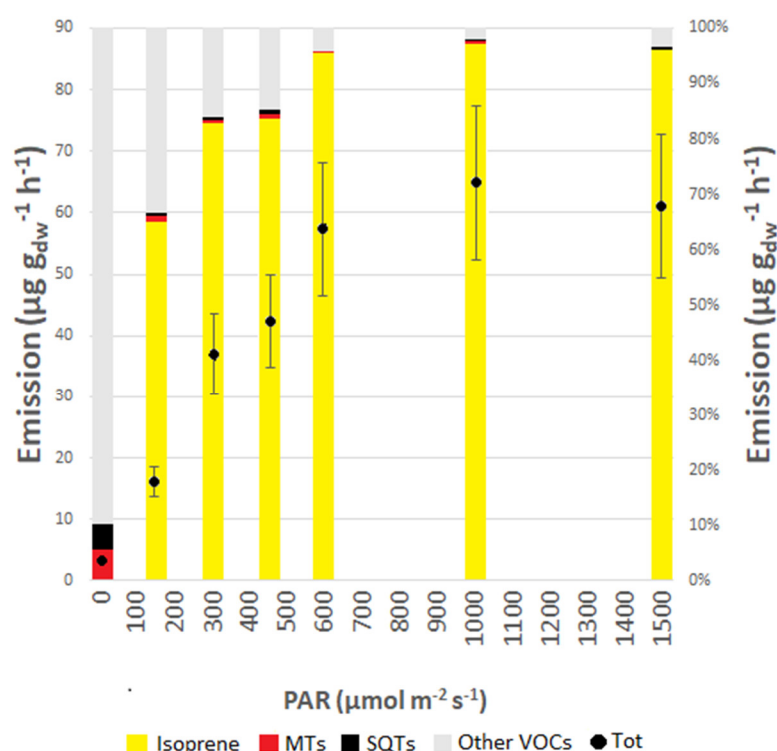
**Table S6.** Values for the fitted STD isoprene curves in Figure S4.  $E_S^p$  is a STD potential emission factor ( $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1}$ ).  $C_T$  was calculated by using mean  $T_c$  for the whole season and year, and  $C_{T1}$ ,  $C_{T1}$ ,  $T_s$  and  $T_M$  adopted from Guenther et al. (1993) [55].

	Lower (z <sub>L</sub> )	Middle (z <sub>M</sub> )	Higher (z <sub>H</sub> )
$E_S^p$ ( $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1}$ )	27.2	118.6	89.6
$C_T$	0.5142	0.3880	0.5207
$\alpha$	0.0093	0.0038	0.0046
$C_{L1}$	4.51	2.92	2.78

$$R_{E/A} = C_{E/A} \frac{\alpha_{E/A} PAR}{\sqrt{1 + \alpha_{E/A}^2 PAR^2}} \quad (\text{S2})$$

**Table S7.** Values for the fitted E/A ratio curves in Figure 4B. The light-dependent part of isoprene (Equation 2) has been adopted and modified.  $C_{E/A}$  (dimensionless) and  $\alpha_{E/A}$  (dimensionless) are constants.

	Lower (z <sub>L</sub> )	Middle (z <sub>M</sub> )	Higher (z <sub>H</sub> )
$C_{E/A}$	0.004	0.004	0.006
$\alpha_{E/A}$	0.0037	0.0026	0.0043



**Figure S5.** Total emission rates ( $\mu\text{g g}_{\text{dw}}^{-1}$ , mean  $\pm$  SD, black circles and left y-axis), and the percentages (stacked bars and right y-axis) for the different BVOC groups at different light levels ( $\mu\text{mol m}^{-2} \text{s}^{-1}$ ) at  $z_M$  ( $n = 6$ ).

$$C_{L,300} = \frac{\alpha C_{L1}(\text{PAR} - 300)}{\sqrt{1 + \alpha^2(\text{PAR} - 300)^2}} \quad (\text{S3})$$

$$C_{L,150} = \frac{\alpha C_{L1}(\text{PAR} - 150)}{\sqrt{1 + \alpha^2(\text{PAR} - 150)^2}} \quad (\text{S4})$$

**Table S8.** Values for the fitted curves in Figure 6A,B using Equation (9) for ocimene and Equation (10) for  $\alpha$ -farnesene instead of Equation (3) in Equation (2).

	ocimene	$\alpha$ -farnesene
$E_s$ ( $\mu\text{g g}_{\text{dw}}^{-1} \text{h}^{-1}$ )	0.10	0.29
$C_T$	0.4471	0.4471
$\alpha$	0.0016	0.0015
$C_{L1}$	3.92	1.18

**Table S9.** Slope ( $A/\text{PAR}$ ,  $\mu\text{mol CO}_2 \text{m}^{-2} \text{s}^{-1} \mu\text{mol}^{-1} \text{m}^2 \text{s}$ ,  $n = 3-6$ ) between different PAR values at different height levels in Figure 7A.



PAR	Lower ( $z_L$ )	Middle ( $z_M$ )	Higher ( $z_H$ )
0–150 $\mu\text{mol m}^{-2} \text{s}^{-1}$	0.0449	0.0465	0.0525
150–300 $\mu\text{mol m}^{-2} \text{s}^{-1}$	0.0159	0.0313	0.0224
300–450 $\mu\text{mol m}^{-2} \text{s}^{-1}$	0.0135	0.0230	0.0183
450–600 $\mu\text{mol m}^{-2} \text{s}^{-1}$	0.0028	0.0004	0.0147
600–1000 $\mu\text{mol m}^{-2} \text{s}^{-1}$	0.0029	0.0061	0.0049
1000–1500 $\mu\text{mol m}^{-2} \text{s}^{-1}$	-0.0001	0.0069	0.0024

**Table S10.** Values for the parameters of the fitted curves in Figure 7A using Equation (6).  $A_d$  and  $A_{\max}$  are mean values ( $n = 2-6$ ) at 0 and 1500  $\mu\text{mol m}^{-2} \text{s}^{-1}$ , respectively.

	Lower ( $z_L$ )	Middle ( $z_M$ )	Higher ( $z_H$ )
$A_d$ ( $\mu\text{mol CO}_2 \text{m}^{-2} \text{s}^{-1}$ )	0.66 (0.28)	-0.21 (0.36)	1.27 (0.21)
$A_{\max}$ ( $\mu\text{mol CO}_2 \text{m}^{-2} \text{s}^{-1}$ )	12.05 (3.01)	21.30 (2.92)	18.10 (4.89)
$\alpha_A$ ( $\text{mol mol}^{-1}$ )	0.0541	0.0437	0.0538