Supplementary information

Impact of meteorological conditions on BVOC emission rate from Eastern Mediterranean vegetation under drought

Qian Li[1], Gil Lerner[1], Einat Bar[2], Efraim Lewinsohn[2], Eran Tas[1]

[1] Institute of Environmental Sciences, The Robert H. Smith Faculty of Agriculture, Food and Environment, The Hebrew University of Jerusalem, P.O. Box 12, Rehovot 7610001, Israel

2 Department of Vegetable Research, Agricultural Research Organization – Newe Ya'ar Center, Israel

* Correspondence to:

Eran Tas, Institute of Environmental Sciences, The Robert H. Smith Faculty of Agriculture, Food and Environment, The Hebrew University of Jerusalem, P.O. Box 12, Rehovot 7610001, Israel

eran.tas@mail.huji.ac.il

S1. Preparation of calibration curve for GC–MS

The calibration curve evaluation was conducted with standards of selected volatile organic compounds (VOCs), including monoterpenes (MTs) and sesquiterpenes (SQTs). Two calibration series were conducted. For each series, different solutions were injected into the same measurement sorbent tubes. Then the linear regression fitting function was evaluated based on calculation of the peak area counts vs. VOC mass (μg). The first-series calibration was applied for six VOCs, where the sampled solution base was mixed with 5 μL of each compound. Among them, *cis*-β-ocimene and β-caryophyllene were detected in our research. In the second series of calibrations, we calibrated α-humulene, germacrene D, and α-farnesene. Some details of the standards for the VOCs are shown in Table S1.

Table S1. Summary of calibration compounds' input.

Compound name	**Density (g mL^{-1})**	**Standard volume added (μL)**
cis-β-Ocimene	0.8	5
β-Caryophyllene	0.905	5
α-Humulene	0.88	5
Germacrene D	0.85	5
α-Farnesene	0.81	5

From the initial solution, we prepared 12 and 7 solutions with different concentrations as summarized in Tables S2 and S3 for the first and second calibration series, respectively.

Table S2. Concentration of solutions for the first-series calibration.

Solution	Volume of solutes	Methanol solvent (µL)	Concentration (ng µL^{-1})	Mass of standard in 4 µL injected in the tube (ng)
GIL-080221	**5 µL**	**500**	**~10,000**	
Sol 1	**100 µL of GIL-080221**	**900**	**1000**	
Sol 2	250 µL of Sol 1	750	250	1000
Sol 3	500 µL of Sol 2	500	125	500
Sol 4	500 µL of Sol 3	500	62.5	250
Sol 5	500 µL of Sol 4	500	31.25	125
Sol 6	500 µL of Sol 5	500	15.625	62.5
Sol 7	500 µL of Sol 6	500	7.8125	31.25
Sol 8	480 µL of Sol 7	520	3.75	15
Sol 9	500 µL of Sol 8	500	1.875	7.5
Sol 10	500 µL of Sol 9	500	0.9375	3.75
Sol 11	533 µL of Sol 10	467	0.5	2
Sol 12	500 µL of Sol 11	500	0.25	1

Table S3. Concentration of solutions for the second-series calibration

Solution	Volume of solutes	Methanol solvent	Concentration (ng µL^{-1})	Mass of standard in 4 µL injected in the tube (ng)
Sol 1			**500**	**2000**
Sol 2	100 µL of Sol 1	100	250	1000
Sol 3	100 µL of Sol 2	100	125	500
Sol 4	100 µL of Sol 3	100	62.5	250
Sol 5	100 µL of Sol 4	100	31.25	125
Sol 6	100 µL of Sol 5	100	15.625	62.5
Sol 7	100 µL of Sol 6	100	7.8125	31.25

The settings of the GC–MS for the standard calibrations are shown in Table S4 and were the same for both series.

Table S4. GC–MS analysis settings for the calibration curve evaluation of selected VOCs.

Sample analysis method	Agilent GC–MSD system (7890A) EI Scan
Column	Restek 10623 Stabilwax
Autosampler	Centri
Injector temperature	250 ºC
Oven temp.	45 ºC (5 min), 5 ºC min^{-1} to 180 ºC, 25 ºC min^{-1} to 250 ºC
Mass range	41–350
Gas	Constant pressure (working with retention time lock for iso-butylbenzene at retention time of 7.5 min)
inj	splitless
Threshold, sampling rate	150, 2
EMV mode	Relative, 70 eV
MS source, quad auxiliary temperature	230 ºC, 150 ºC, 280 ºC
Tube – desorption time desorption temperature	5 min 280 ºC
Trap – desorption time desorption temperature	3 min (20 °C s^{-1} to 300 °C) 300 ºC

The calibration curve results are presented in Figs. S1–S5, and are summarized in Table S5.

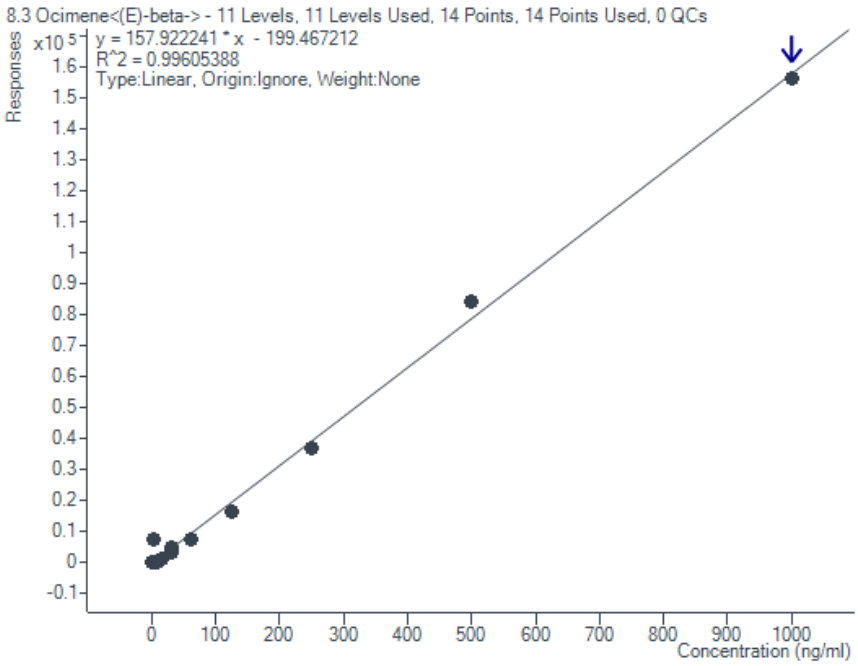

Figure S1. Calibration curve for β-ocimene (E)

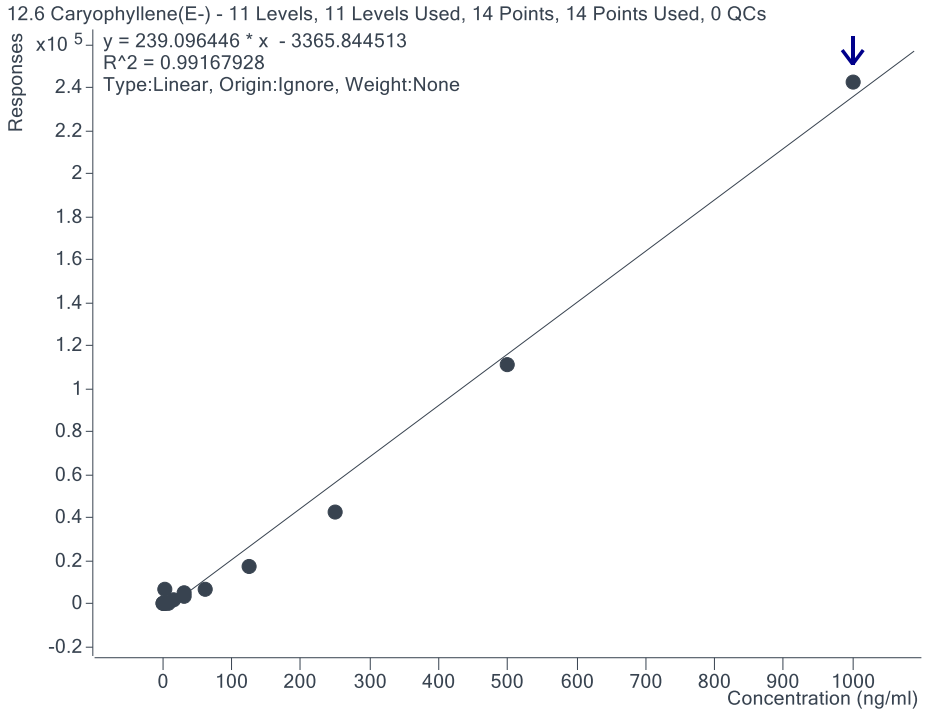

Figure S2. Calibration curve for β-caryophyllene

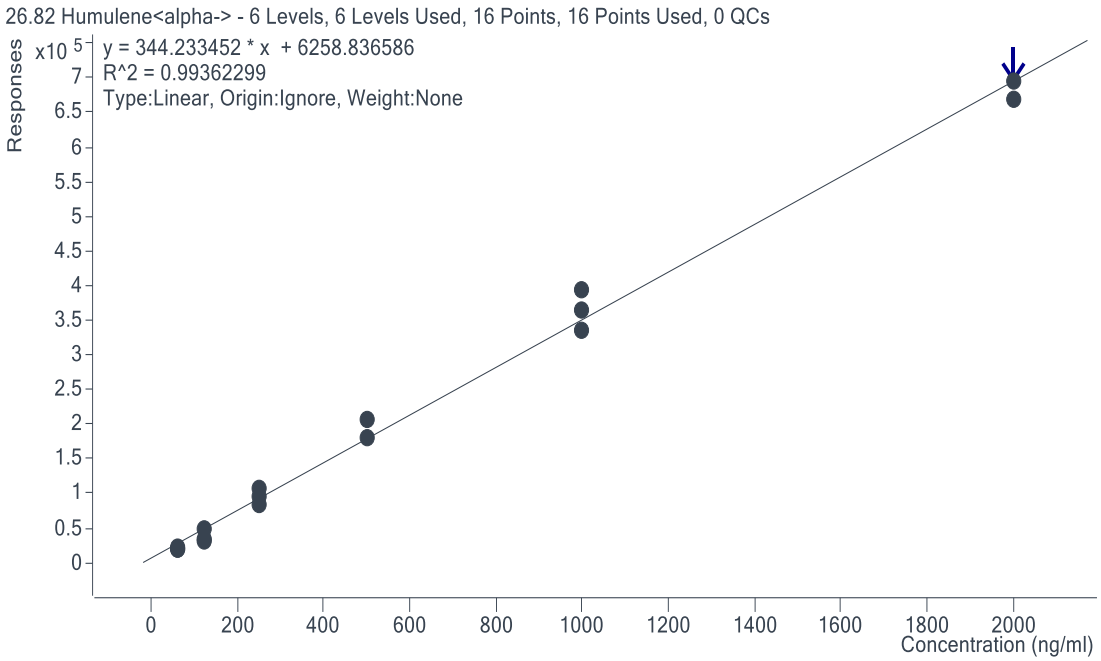

Figure S3. Calibration curve for α-humulene

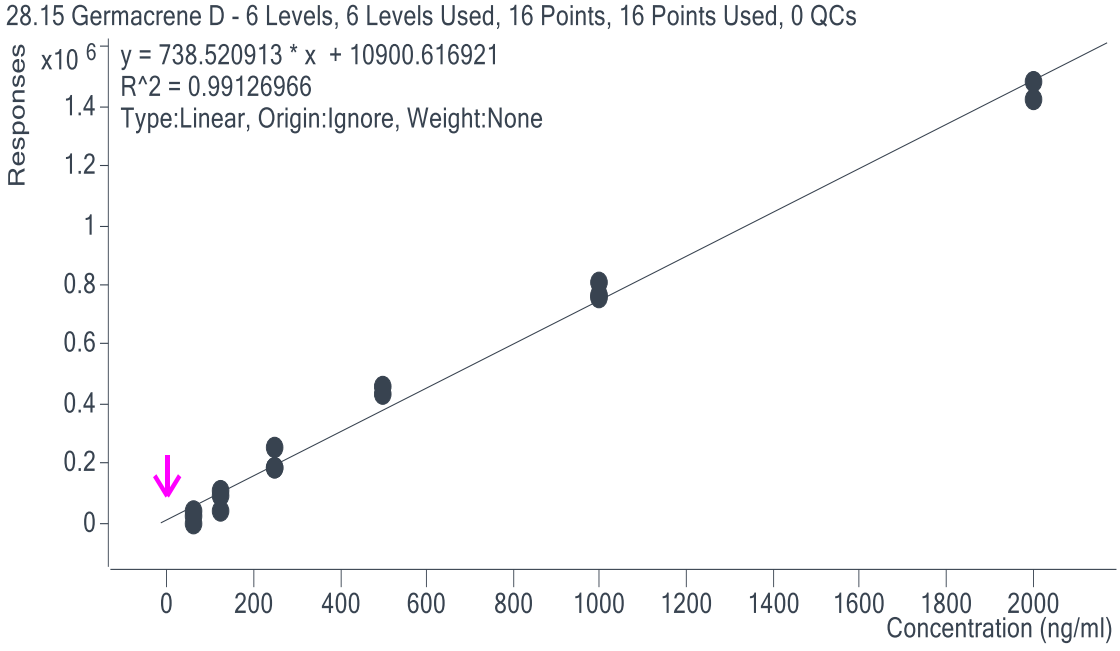

Figure S4. Calibration curve for germacrene D

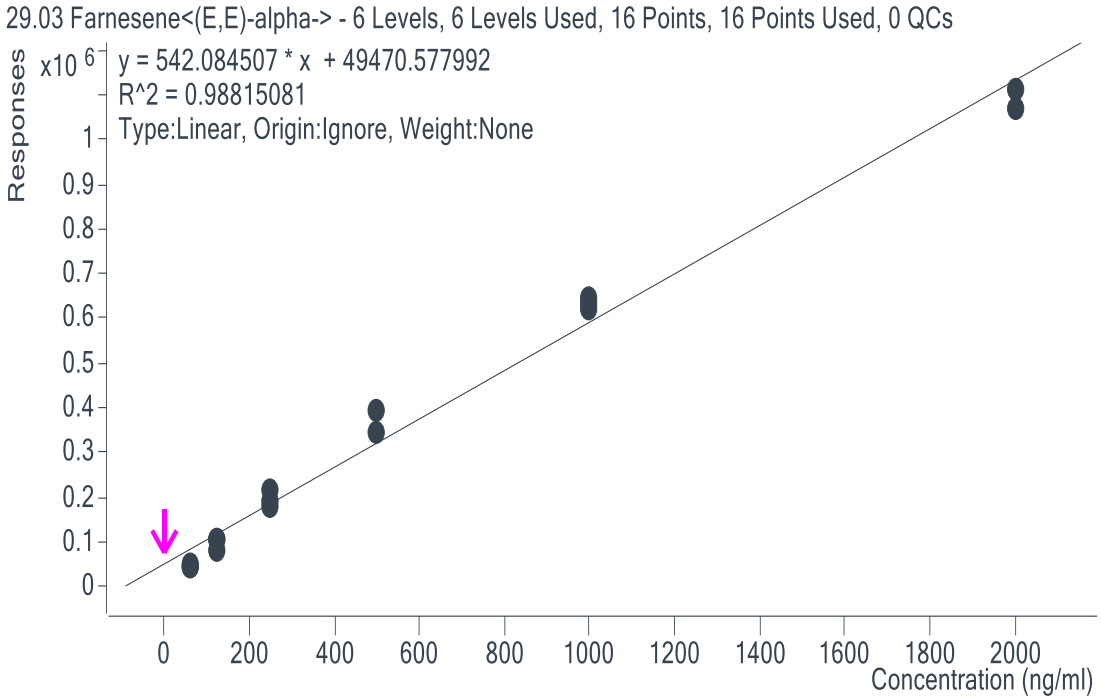

Figure S5. Calibration curve for α-farnesene

Table S5. Regression equations for the five VOC compounds' standard calibration curves

VOC compound name	**r^2**	**Regression equation**
E-β-ocimene	0.996	y = 157.9220 * x -199.46
β-Caryophyllene	0.991	y =239.096 * x - 3365.84
α-Humulene	0.993	y = 344.233452 * x + 6258.836586
Germacrene D	0.991	y = 738.626951 * x - 4579.005169
α-Farnesene	0.994	y = 617.012200 * x + 22800.770090

S2. Linear and hyperbolic correlation between MTs/SQTs and (temporal changes in RH (δ_{RH}))

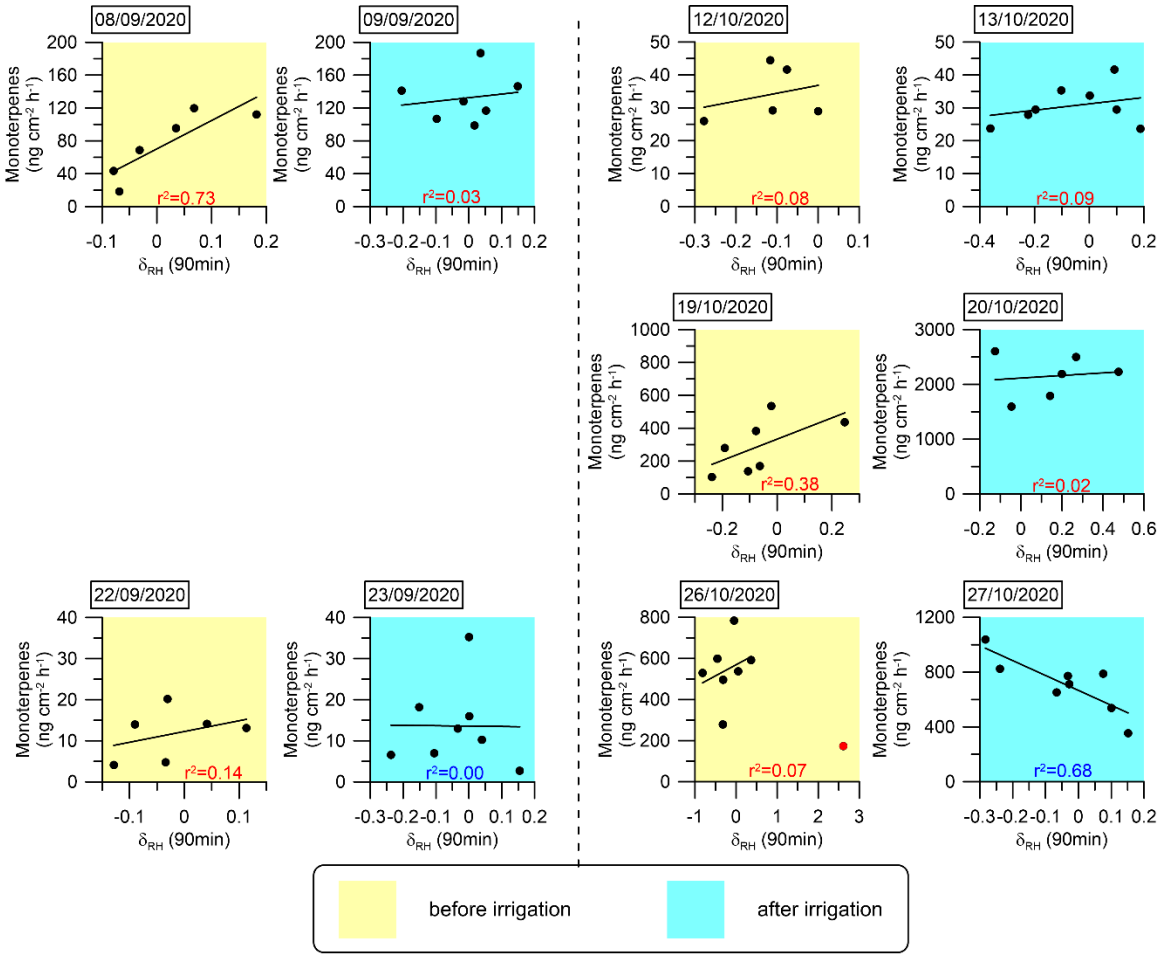

Figure S6. Daily correlations between MT emission fluxes and δ_{RH}. A linear fitting function is used for the fitting curves. The coefficient of determination (r^2) for each day is marked in red or blue when the correlation is positive or negative, respectively.

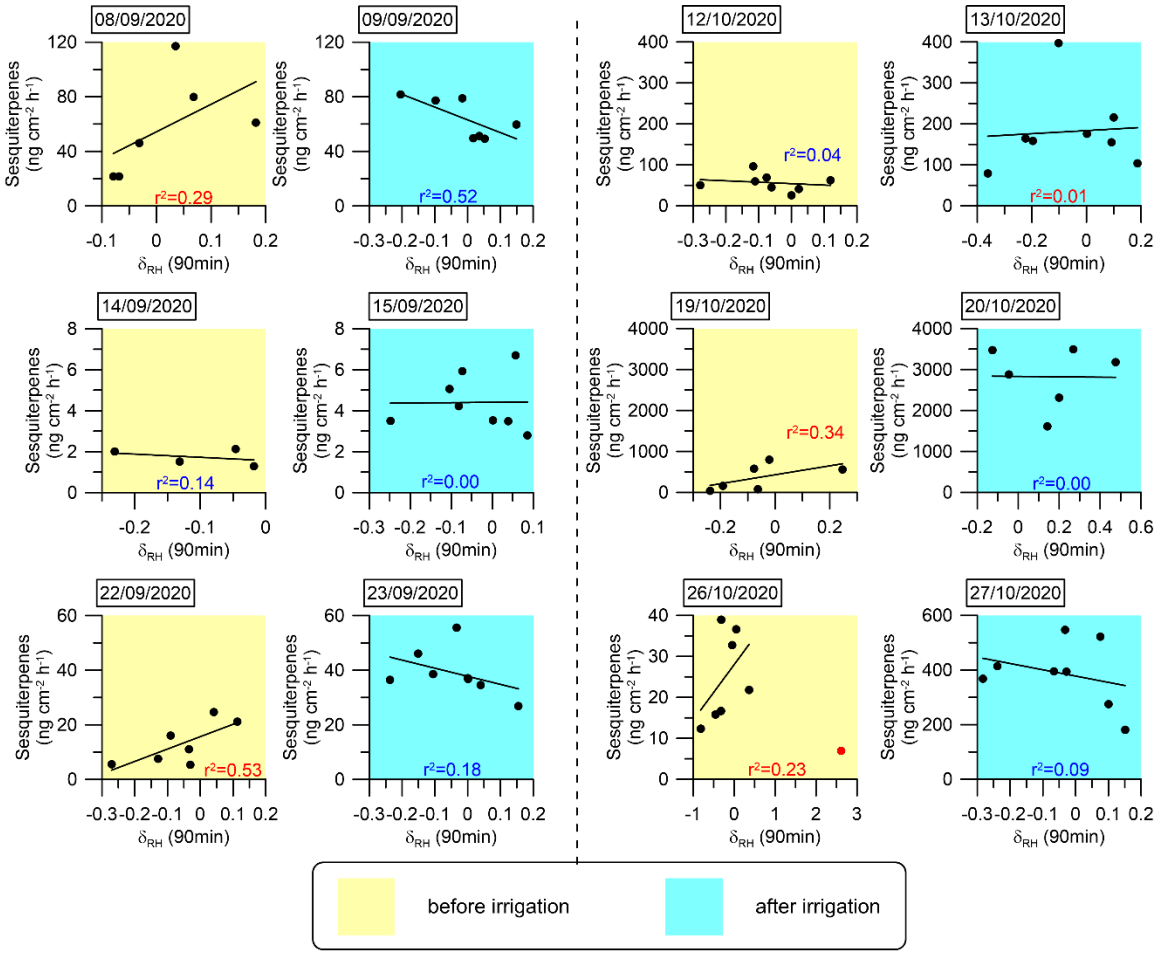

Figure S7. Daily correlations between SQT emission fluxes and δ_{RH}. A linear fitting function is used for the fitting curves. The coefficient of determination (r^2) for each day is marked in red or blue when the correlation is positive or negative, respectively. The sample at 12:10 h on 26 Oct 2020 (marked in red) was not considered in the fitting curve for that day, because an extremely sharp increase in RH (from 10 to 31%) occurred within 10 min, which we considered an outlier.

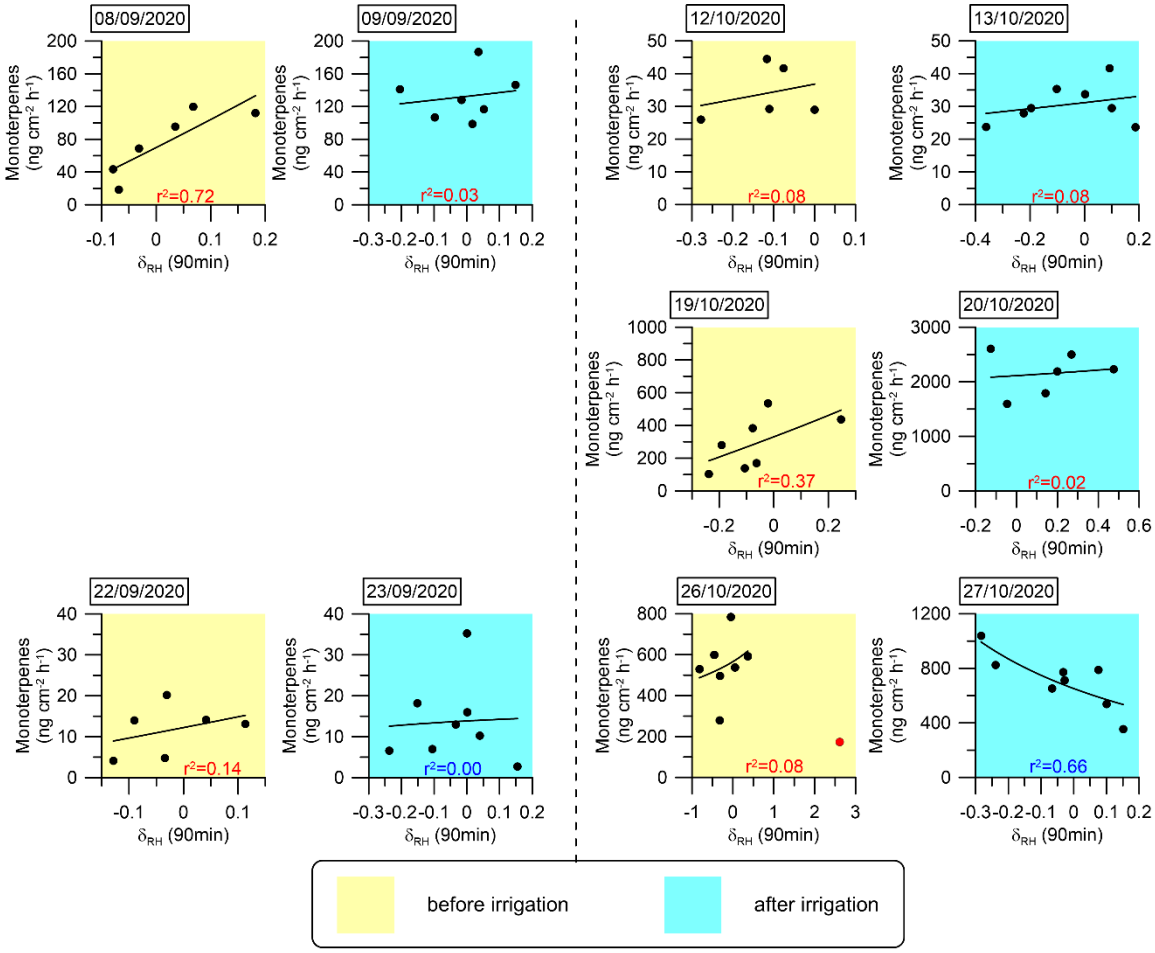

Figure S8. Daily correlations between MT emission fluxes and δ_{RH}. A hyperbolic fitting function was used for the fitting curves. The coefficient of determination (r^2) for each day is marked in red or blue when the correlation is positive or negative, respectively.

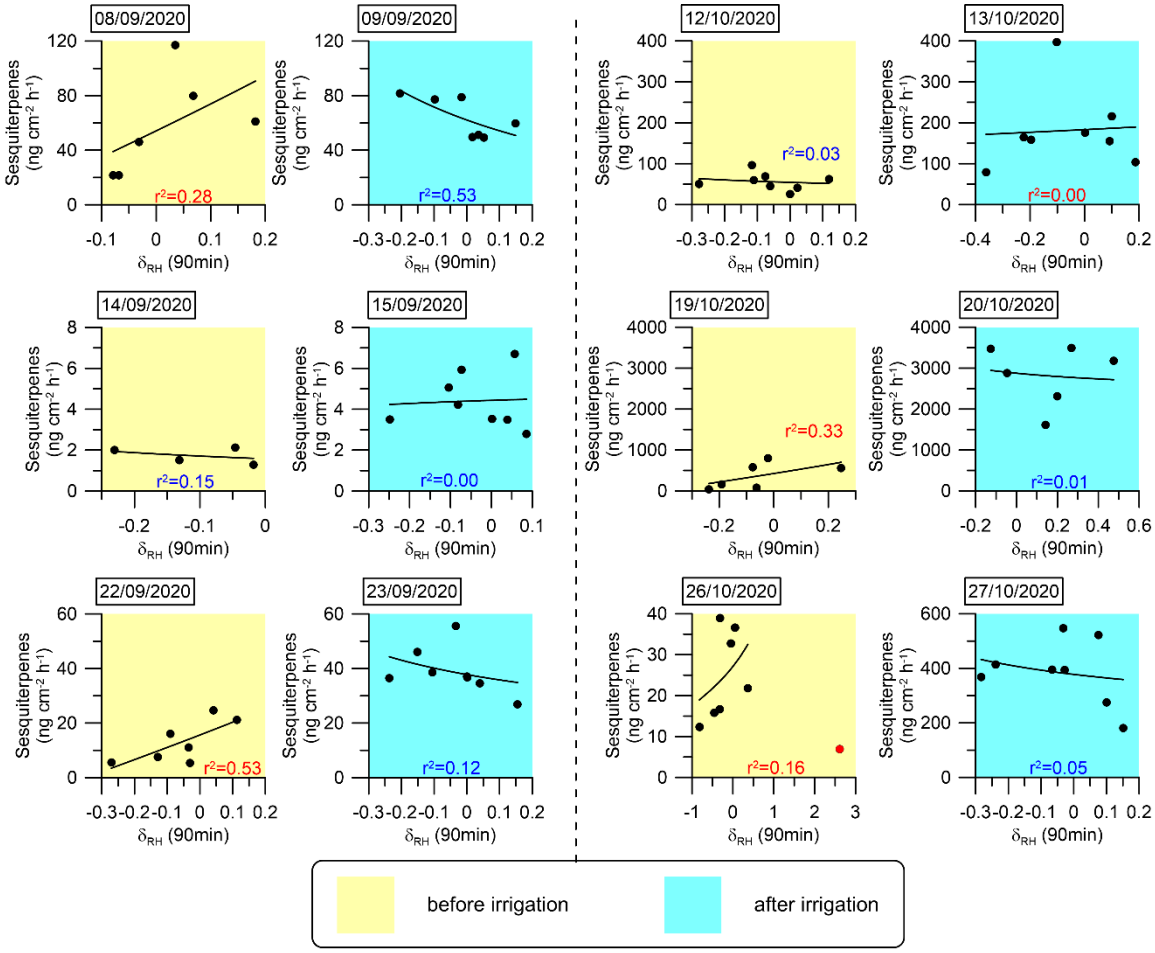

Figure S9 Daily correlations between SQT emission fluxes and δ_{RH}. A hyperbolic fitting function was used for the fitting curves. The coefficient of determination (r^2) for each day is marked in red or blue when the correlation is positive or negative, respectively. The sample at 12:10 h on 26 Oct 2020 (marked in red) was not considered in the fitting curve for that day, because an extremely sharp increase in RH (from 10 to 31%) occurred within 10 min, which we considered an outlier.

S3. Exponential correlation between MTs/SQTs and RH

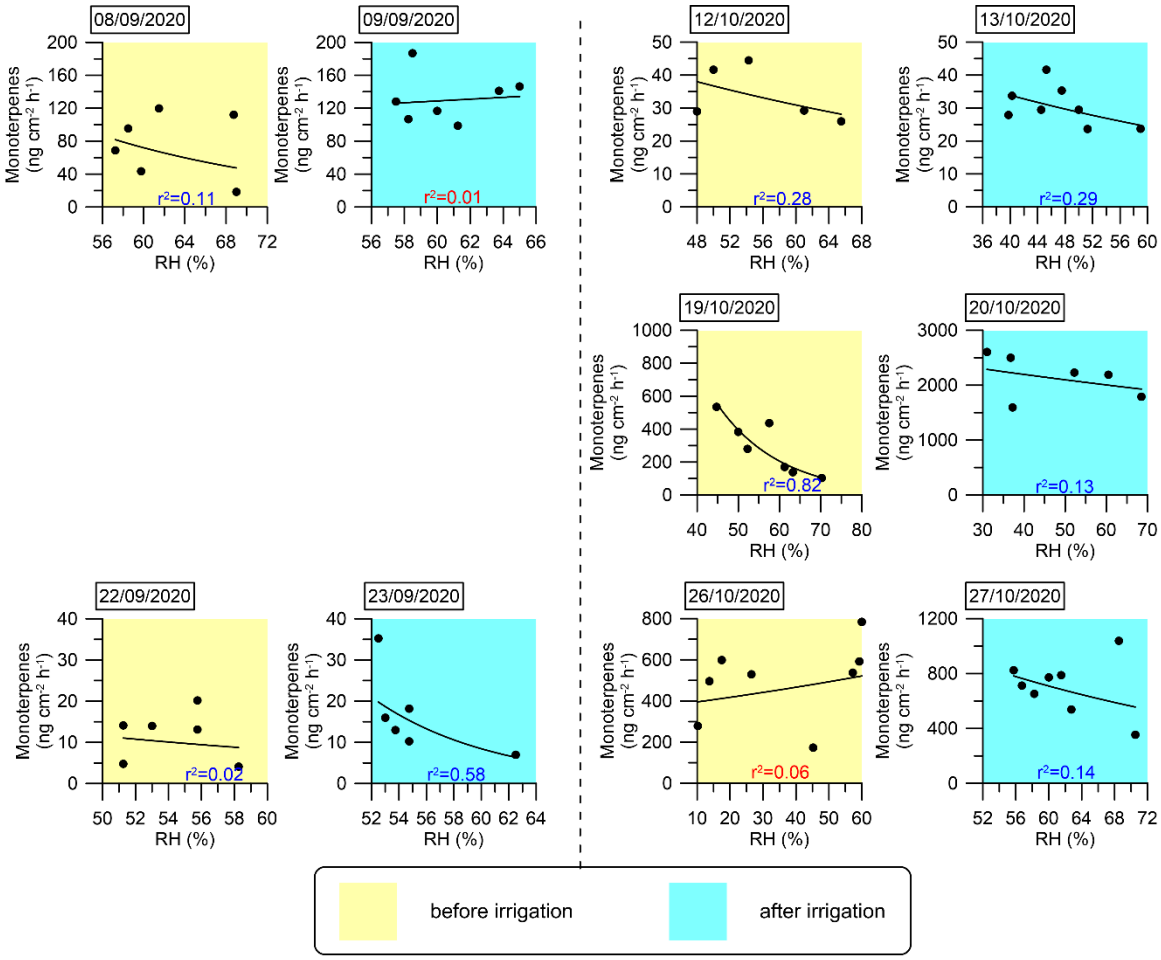

Figure S10. Daily correlations between MT emission fluxes and RH. A linear fitting function was used for the fitting curves. The coefficient of determination (r^2) for each day is marked in red or blue when the correlation is positive or negative, respectively.

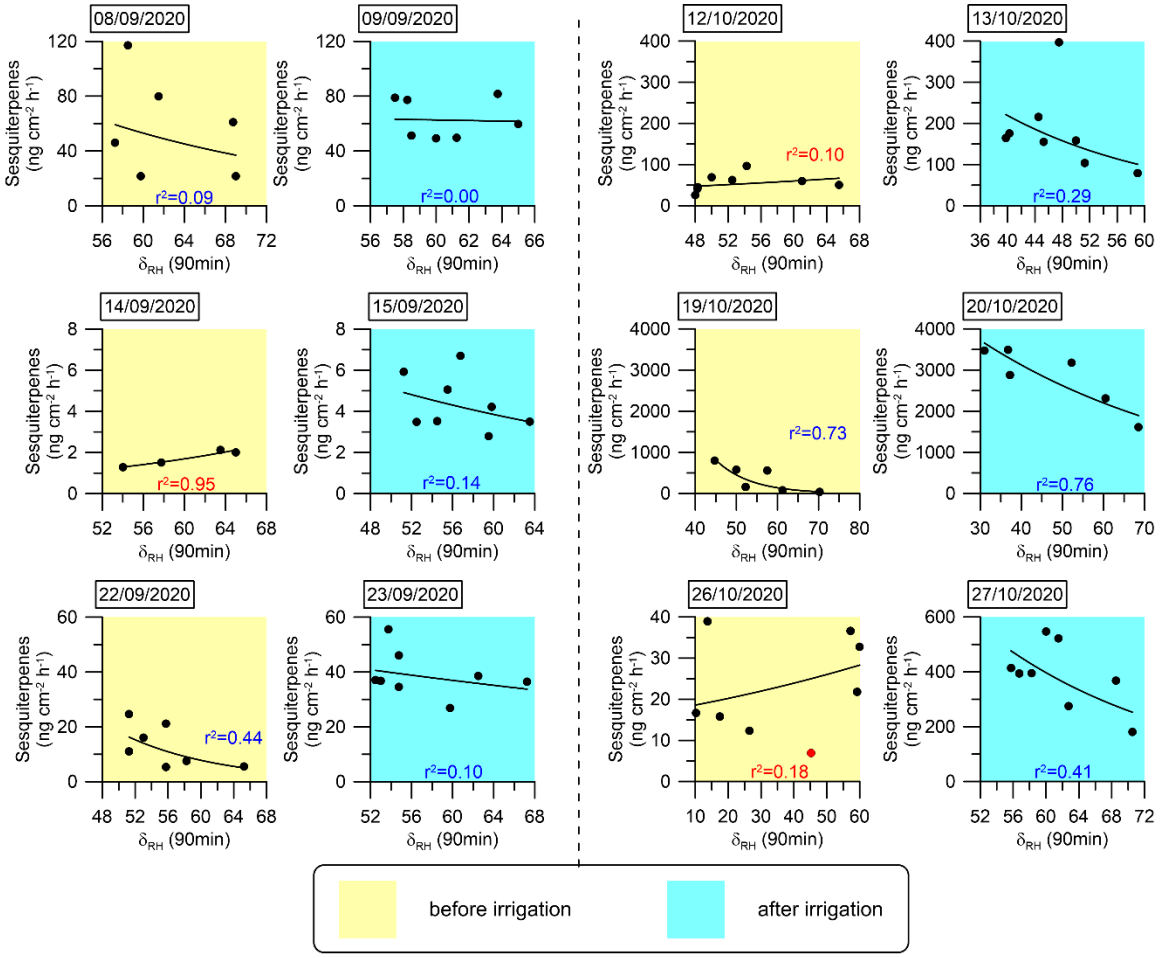

Figure S11. Daily correlations between SQT emission fluxes and RH. A linear fitting function was used for the fitting curves. The coefficient of determination (r^2) for each day is marked in red or blue when the correlation is positive or negative, respectively. The sample at 12:10 h on 26 Oct 2020 (marked in red) was not considered in the fitting curve for that day, because an extremely sharp increase in RH (from 10 to 31%) occurred within 10 min, which we considered an outlier.