Supplementary Material for

Insights into the Intraspecific Variability of the Above and Belowground Emissions of Volatile Organic Compounds In Tomato

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Supplementary Figures S1 and S2 Supplementary Tables S1 and S2

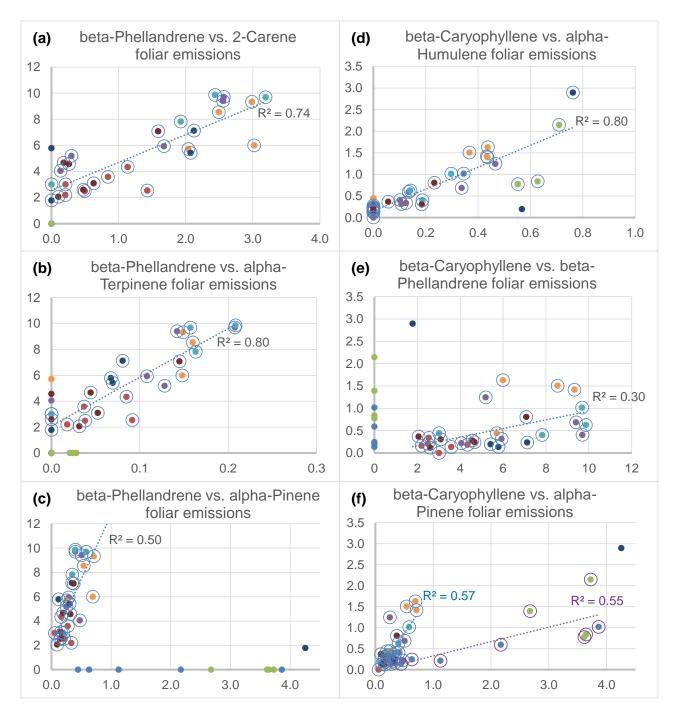


Figure S1. Examples of covariations between individual VOCs emitted by tomato foliage. Data points show measurements of single plant replicates across all genotypes (emission rates in ng m⁻² projected leaf surface s⁻¹). Different colors correspond to the different tomato genotypes as shown in Figure 3(**b**). Lines and coefficients of determination R² show the results from Pearson correlations. Data points without open circles were excluded from the correlation analyses. Generally, the emissions of all individual monoterpenes were correlated with each other except linalool, whose emissions were unrelated to the emissions of other VOCs. The strongest correlations were found between the MTs β-phellandrene, δ-2-carene and α-terpinene (R²: 0.70–0.80, examples shown in (**a**), (**b**)), whereas correlations with pinenes were more moderate (R²: 0.50–0.57, example shown in (**c**)). The emissions of the major sesquiterpene β-caryophyllene were well correlated with the emissions of its structural isomer α-humulene (R²: 0.80, (**d**)), and poorly or moderately with major monoterpenes ((R²: 0.30–0.57, examples shown in (**e**), (**f**)). Note that two genotypes (Cervil, Plovdiv) did not emit β-phellandrene and δ-2-carene but larger amounts of α- and β-pinene compared to the other genotypes.

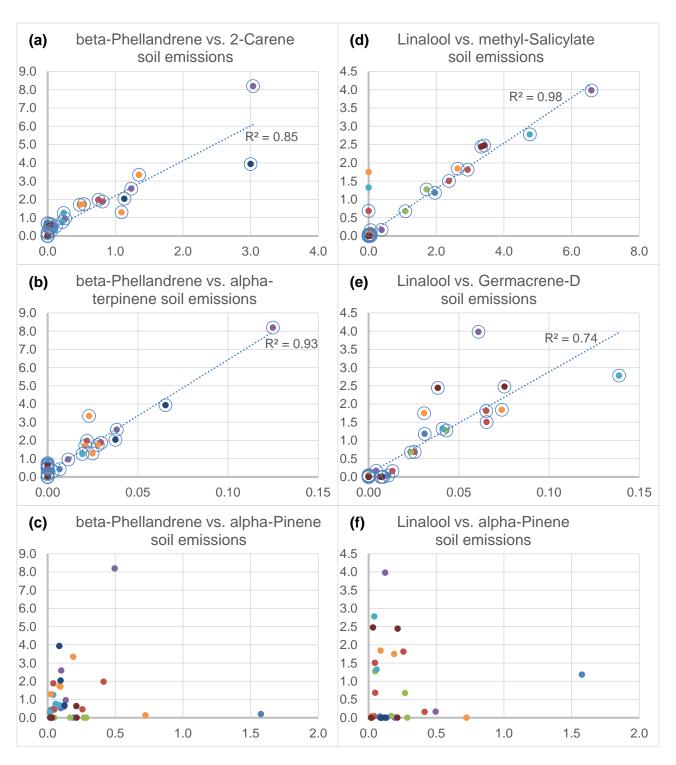


Figure S2. Examples of covariations among soil emissions (ng m⁻² soil surface s⁻¹) of individual VOCs across all genotypes. Different colors correspond to the different tomato genotypes as shown in Figure 3(**b**). Pearson correlation analyses with resulting coefficients of determination R² were made on the data with open circles. Generally, there were two groups of VOCs, within each one individual emissions were correlated: group 1 consisted of β-phellandrene, δ-2-carene, α-terpinene, α-phellandrene, p-cymene and terpinolene, examples shown in (**a**), (**b**), and group 2 of linalool, methyl-salicylate and most sesquiterpenes examples shown in (**d**), (**e**). Soil emissions of α- and β-pinene were unrelated to other VOCs examples shown in (**c**), (**f**).

Table S1. List of VOCs analyzed by GC-MS that were observed either in the emissions from foliage and/or soil and/or in the extracts of leafs and/or roots. The occurrence of each compound is indicated below the compound name as follows: Emission from Foliage: E/F; Emission from Soil with Plant: E/S+P; Emission from Soil without Plants: E/S-P; Content in Leaves (leaf extract): C/L; Content in Roots (root extract): C/R. VOC classes: MT: non-oxygenated monoterpenes; oxMT: oxygenated monoterpenes; SQT: non-oxygenated sesquiterpenes; oxSQT: oxygenated sesquiterpenes; Phenolic: Phenolic compound (benzenoïds and phylpropanoïds); OVOC: other oxygenated compounds. * Tentative identification; ND Not Detected; \$Adams (2005), NIST 2005, Wiley 2009.

| Compound (occurrence) | Formula (Molecular weight) | Assigned VOC class | Retention Time | Retention Index | Retention Time | Retention Index | Reference Retention Index ^{\$} | |
|---|----------------------------------|-----------------------|-------------------|--------------------|-------------------|-------------------------|---|--|
| | | | GC-MS analy | sis emissions | GC-MS ana | GC-MS analysis extracts | | |
| Hexanal E/S-P | C6H12O (100) | OVOC | 5.43 | 796 | ND | ND | 801 | |
| Nonene E/S-P | C9H18 (126) | OVOC | 8.42 | 889 | ND | ND | 891 | |
| Heptanal E/S-P | C7H14O (114) | OVOC | 8.7 | 898 | ND | ND | 901 | |
| α-Pinene E/F, E/S+P, C/L | C10H16 (136) | MT | 9.81 | 933 | 11.02 | 939 | 932 | |
| 3-Octen-ol* E/S+P, E/S-P | C8H16O (128) | OVOC | 10.87 | 965 | ND | ND | 974 | |
| β-Pinene E/F, E/S+P | C10H16 (136) | MT | 11.18 | 975 | ND | ND | 974 | |
| 6-methyl-5- heptanone* E/S+P, E/S-P | C8H14O (126) | OVOC | 11.44 | 983 | ND | ND | 981 | |
| β-Myrcene E/F, E/S+P, C/L | C10H16 (136) | MT | 11.68 | 990 | 13.54 | 977 | 988 | |
| Octanal E/S-P | C8H16O (128) | OVOC | 11.9 | 996 | ND | ND | 998 | |
| δ-2-Carene E/F, E/S+P, C/L | C10H16 (136) | MT | 11.91 | 997 | 14.25 | 988 | 1001 | |
| α- Phellandrene E/F, E/S+P | C10H16 (136) | MT | 12.08 | 1002 | ND | ND | 1002 | |
| unknown monoterpene E/S+P, E/S-P | C10H16 (136) | MT | 12.3 | 1009 | ND | ND | | |
| α-Terpinene E/F, E/S+P | C10H16 (136) | MT | 12.47 | 1015 | ND | ND | 1014 | |
| p-Cymene E/F, E/S+P β- | C10H14 (134) | MT | 12.7 | 1022 | ND | ND | 1020 | |
| Phellandrene E/F, E/S+P, C/L, C/R | C10H16 (136) | MT | 12.88 | 1027 | 15.5 | 1025 | 1025 | |
| Hexanoic acid E/S+P, E/S-P | C8H18O (130) | OVOC | 12.89 | 1028 | ND | ND | 1027 | |

| DI 1 . 11 | | | | | | | |
|---|-------------------|----------|-------|------|-------|------|------|
| Phenylacetald ehyde C/R | C7H8O (108) | Phenolic | ND | ND | 15.68 | 1039 | 1036 |
| β-Ocimene E/F, E/S+P (Z)-2,6- | C10H16 (136) | MT | 13.47 | 1046 | ND | ND | 1044 |
| dimethyl-2,6- Octadiene* | C10H18 (138) | MT? | 13.58 | 1050 | ND | ND | 978 |
| γ-Terpinene E/F, E/S+P, E/S-P | C10H16 (136) | MT | 13.82 | 1058 | ND | ND | 1054 |
| Acetophenone E/S-P | C8H8O (120) | Phenolic | 13.9 | 1060 | ND | ND | 1059 |
| Octanol E/S-P | C8H18O (130) | OVOC | 14.26 | 1069 | ND | ND | 1060 |
| Terpinolene E/F, E/S+P | C10H16 (136) | MT | 14.76 | 1087 | ND | ND | 1085 |
| o-Guaiacol C/R | C7H8O2 (124) | Phenolic | ND | ND | 17.59 | 1079 | 1087 |
| Unknown Aldehyde C/R | C10H16O (152) | oxMT? | ND | ND | 18.33 | 1094 | |
| Linalool E/F, E/S+P, E/S-P | C10H18O (154) | oxMT | 15.04 | 1096 | ND | ND | 1095 |
| Nonanal E/S-P | C9H18O (142) | OVOC | 15.11 | 1098 | ND | ND | 1100 |
| unknown compound E/S+P, E/S-P | C10H20O (156) | ? | 15.53 | 1111 | ND | ND | |
| Octanoic acid E/S-P | C18H16O2 (144) | OVOC | 17.44 | 1175 | ND | ND | 1167 |
| Methyl salicylate E/S+P, C/L, C/R | C8H8O3 (152) | Phenolic | ND | ND | 22.99 | 1170 | 1190 |
| Decanal E/S-P | C10H20O (156) | OVOC | 18.14 | 1199 | ND | ND | 1201 |
| Geraniol C/R | C10H18O (154) | oxMT | ND | ND | 25.9 | 1228 | 1249 |
| Nonanoic acid E/S-P | C9H18O (142) | OVOC | 20.05 | 1262 | ND | ND | 1267 |
| Undecanal E/S-P | C11H22O (170) | OVOC | 21.06 | 1301 | ND | ND | 1305 |
| δ-Elemene E/F, E/S+P, E/S-P, C/L | C15H24 (204) | SQT | 22.11 | 1341 | 30.35 | 1335 | 1335 |
| Eugenol C/L | C10H12O2 (164) | Phenolic | ND | ND | 30.58 | 1350 | 1356 |
| (E)-β- Caryophyllene E/F, E/S+P, C/L | C15H24 (204) | SQT | 24.34 | 1426 | 34.93 | 1421 | 1417 |
| Geranylaceton e E/S-P | C13H22O (194) | oxMT | 24.92 | 1449 | ND | ND | 1453 |
| | | | | | | | |

| α-Humulene E/F, E/S+P, E/S-P | C15H24 (204) | SQT | 25.2 | 1461 | ND | ND | 1452 |
|------------------------------------|-------------------|--------|-------|------|----|----|------|
| Dodecanol E/S+P, E/S-P | C12H26O (186) | OVOC | 25.51 | 1473 | ND | ND | 1469 |
| Germacrene D E/F, E/S+P | C15H24 (204) | SQT | 25.87 | 1487 | ND | ND | 1484 |
| Pentadecane E/S-P | C15H32 (212) | OVOC | 26.2 | 1500 | ND | ND | 1500 |
| Dodecanoic acid E/S-P | C12H24O2 (200) | OVOC | 27.66 | 1561 | ND | ND | 1565 |
| Germacrene-4- ol* E/F | C15H26O (222) | oxSQT? | 27.75 | 1565 | ND | ND | 1574 |
| Unknown SQT E/F, E/S-P | C15H24 (204) | SQT | 28.07 | 1578 | ND | ND | |
| Tetradecanal E/S+P, E/S-P | C14H28O (212) | 212 | 28.75 | 1606 | ND | ND | 1611 |
| | | | | | | | |

Table S2. Emission rates (mean \pm SE, n = 4-6) of individual major VOCs, sum of major VOCs, sum of all monoterpenes, sum of all sesquiterpenes and sum of all compounds measured under light and dark conditions on the eight parents of the tomato MagicTom population. Please, refer to Table S1 above for the identification of minor monoterpenes and sesquiterpenes. P-values in the right column denote the significance levels for the effect of genotype based on ANOVA or Kruskall-Wallis tests (considered as significant at p < 0.05). Superscript letters indicates the significant differences among the individual genotypes resulting from pairwise-comparisons with Bonferroni or Dunn tests. ND: Not Detected.

| VOC | Cervil | Criolo | Plovdiv | LA1420 | LA0147 | Ferum | Levovil | Stupicke | P-value |
|----------------|------------------------|-------------------------|-------------------------|--------------------------|--------------------------|---------------------------|--------------------------|-------------------------|---------------------|
| α-Pinene | 1.65 ±0.58bc | 0.20±0.04ª | 3.42±0.20° | 0.38±0.05 ^{abc} | 0.38±0.07 ^{abc} | 0.55 ±0.09 ^{abc} | 1.26±0.81 ^{abc} | 0.22±0.04 ^{ab} | 0.002\$ |
| | 0.56±0.10 ^a | 0.24±0.14a | 1.07±0.25a | 0.17±0.03a | 0.37 ± 0.07^{a} | 0.50 ± 0.27^{a} | 0.27 ±0.10 ^a | 0.09 ± 0.02^{a} | 0.041\$ |
| δ-2-Carene | 0.00±0.00a | 0.72±0.20 ^{ab} | 0.00±0.00a | 1.45 ± 0.48^{ab} | 1.89 ± 0.56^{ab} | 2.63 ±0.19b | 1.05 ± 0.50^{ab} | 0.54 ± 0.22^{ab} | 0.002\$ |
| | 0.00±0.00a | 0.11 ± 0.07^{ab} | 0.00±0.00a | 0.83±0.31ab | 1.94±0.54b | 0.50 ± 0.14^{ab} | 0.25 ±0.05ab | 0.12±0.05ab | 0.009\$ |
| β-Phellandrene | 0.00±0.00a | 3.03 ±0.33ab | 0.00±0.00a | 6.86 ± 1.04^{b} | 7.60±1.30 ^b | 7.39 ± 0.74^{b} | 5.03 ±0.93ab | 4.01 ± 0.75^{ab} | < 0.001 \$ |
| | 0.00±0.00a | 1.20±0.11 ^{ab} | 0.00±0.00a | 3.26±0.79ab | 5.63±1.02b | 3.16±0.56ab | 1.53 ±0.45ab | 1.22±0.40ab | 0.002\$ |
| Linalool | 2.42±0.92 | 0.30 ± 0.30 | 0.00 ± 0.00 | 1.78 ± 1.44 | 3.45 ± 1.82 | 1.31 ±1.07 | 0.02 ± 0.01 | 2.11 ± 0.72 | 0.246\$ |
| | ND | ND | ND | ND | ND | ND | ND | ND | - |
| (E)-β- | 0.44 ± 0.15^{ab} | 0.17±0.05a | 1.29±0.26 ^b | 0.57±0.17 ^{ab} | 0.62±0.11ab | 1.25 ±0.22b | 0.87±0.55ab | 0.35 ± 0.10^{ab} | 0.007\$ |
| Caryophyllene | 0.40±0.11ab | 0.14±0.04a | 0.75 ±0.04 ^b | 0.17±0.02ab | 0.44±0.08ab | 0.21 ±0.02ab | 0.36±0.16ab | 0.23±0.06ab | 0.061\$ |
| Sum of major | 4.51±0.45a | 4.42±0.59a | 4.70±0.33ab | 11.06±1.16 ^{ab} | 13.93±1.24b | 13.13±0.54b | 8.21 ±0.67ab | 7.23 ± 0.87^{ab} | < 0.001\$ |
| VOCs | 0.95±0.17 ^a | 1.69±0.20 ^{ab} | 1.82±0.23ab | 4.43±1.12ab | 8.38±1.64b | 4.37±0.82ab | 2.41 ±0.72ab | 1.96±0.45ab | 0.021\$ |
| Sum of Mono- | 4.43±0.42° | 4.53±0.63° | 6.20±0.96° | 11.17±1.35 ^{ab} | 14.69±1.29a | 13.48±0.38a | 7.95±0.68bc | 7.12±0.85 ^{bc} | <0.001 £ |
| terpenes | 0.77±0.13 ^a | 2.07±0.43ab | 1.13±0.26 ^{ab} | 4.53 ±1.22ab | 9.39±1.81 ^b | 4.85±0.94ab | 2.67 ±0.80ab | 1.79±0.48ab | 0.009\$ |
| Sum of Sesqui- | 0.67 ± 0.26^{a} | 0.71±0.20a | 2.34±0.31a | 2.17±0.71a | 1.01 ±0.21a | 2.10±0.36a | 1.60±0.80a | 1.10±0.21a | 0.087 [£] |
| terpenes | 0.63±0.15 | 0.63±0.24 | 1.36±0.04 | 0.98±0.46 | 0.74 ± 0.13 | 0.38±0.03 | 0.74 ± 0.26 | 0.57 ± 0.14 | 0.422\$ |
| Sum of all | 5.10±0.45° | 5.24±0.77° | 8.54±0.87 ^{bc} | 13.34±1.60 ^{ab} | 18.70±1.42a | 15.59±0.44a | 9.55±0.95 ^{bc} | 8.22±0.91° | <0.001 [£] |
| VOCs | 1.40±0.26a | 2.70±0.66ab | 2.50±0.23ab | 5.51 ±1.56ab | 10.13±1.91b | 5.23 ±0.98ab | 3.43 ±1.03 ^{ab} | 2.36±0.47ab | 0.022\$ |

[£] ANOVA plus Bonferroni post-hoc tests; ^{\$} Kruskall-Wallis plus Dunn's test