

**Table S1.** Detailed environmental data on collection sites.

| Label <sup>a</sup> | T. min <sup>b</sup> | T. max <sup>c</sup> | Precipitation <sup>d</sup> | Rad. <sup>e</sup> | Ratio <sup>f</sup> | Lithology <sup>g</sup> | Vegetation <sup>h</sup>               |
|--------------------|---------------------|---------------------|----------------------------|-------------------|--------------------|------------------------|---------------------------------------|
| BAO                | 2                   | 10                  | 138                        | 8.3               | 41.75              | Metamorphic rocks      | Forest clearing ( <i>Quercus</i> sp.) |
| CAM                | 8                   | 15                  | 71.75                      | 9.05              | 14.25              | Alluvial deposits      | Forest clearing ( <i>Pinus</i> sp.)   |
| DOM                | 5                   | 13                  | 109.25                     | 9.3               | 14.25              | Metamorphic rocks      | Forest clearing ( <i>Quercus</i> sp.) |
| JER                | 4                   | 12                  | 65.5                       | 9.3               | 19.25              | Metamorphic rocks      | Mediterranean shrub                   |
| SIS                | 8                   | 15                  | 40.5                       | 10                | 6.75               | Marls                  | Abandoned agricultural lot            |
| SUP                | 8                   | 15                  | 35.5                       | 10                | 6.75               | Marls                  | Degraded urban lot                    |

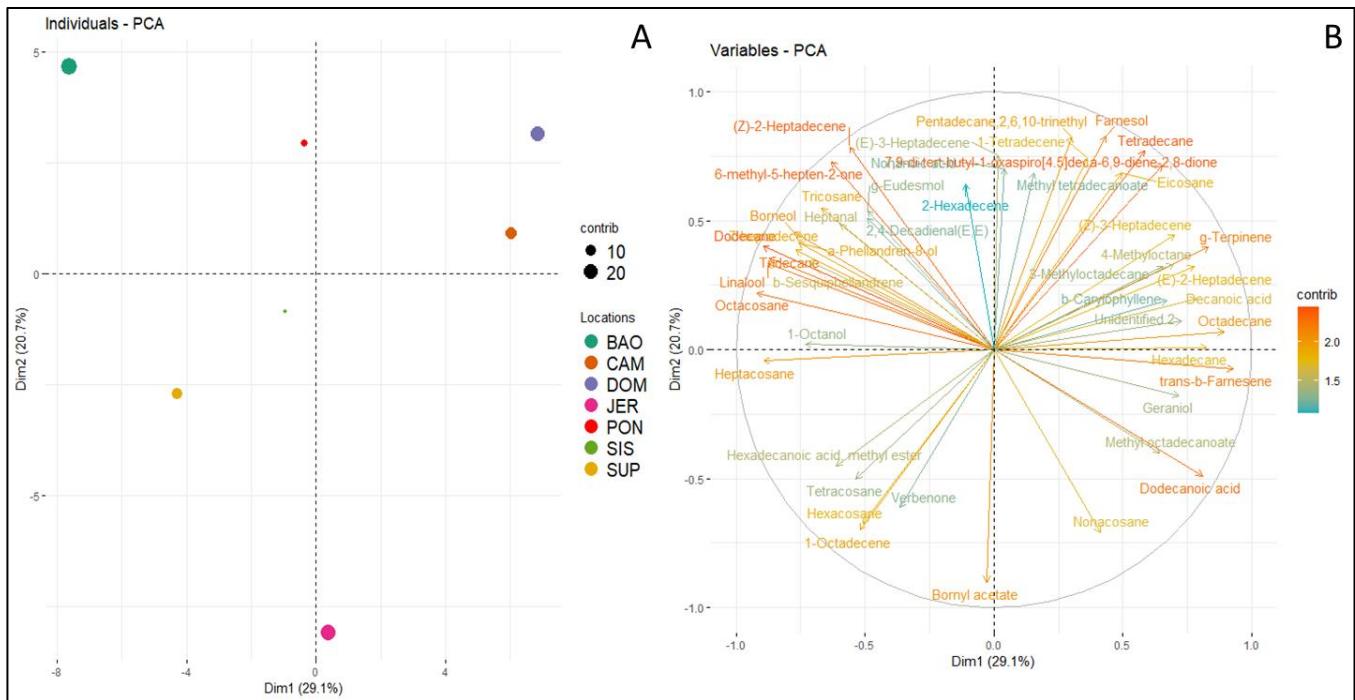
<sup>a</sup>Acronyms used to refer to the studied populations (BAO= Bau Onu, CAM= Capo Mannu, DOM= Domusnovas, JER= Jerzu, SIS= Sant'Isidoro, SUP= Su Planu); <sup>b</sup>mean value of the daily minimum temperature (°C); <sup>c</sup>mean value of the daily maximum temperature (°C); <sup>d</sup>precipitations (mm); <sup>e</sup>solar radiation (MJ/m2); <sup>f</sup>precipitation to temperature ratio; <sup>g</sup>lithological framework; <sup>h</sup>vegetation. The source of climatological, lithological and vegetational data are reported in the main text as [15-17].

**Table S2.** Integration table to Figure 4. The list of compounds shared by populations (BAO= Bau Onu, CAM= Capo Mannu, DOM= Domusnovas, JER= Jerzu, SIS= Sant'Isidoro, SUP= Su Planu) is reported in the first column. The second column reports the number of populations sharing compounds in each group, the number of compounds shared and the percentage in relation to the total number of compounds identified. The red letter preceding the list of populations refers to the areas in the Venn diagram (Figure 4).

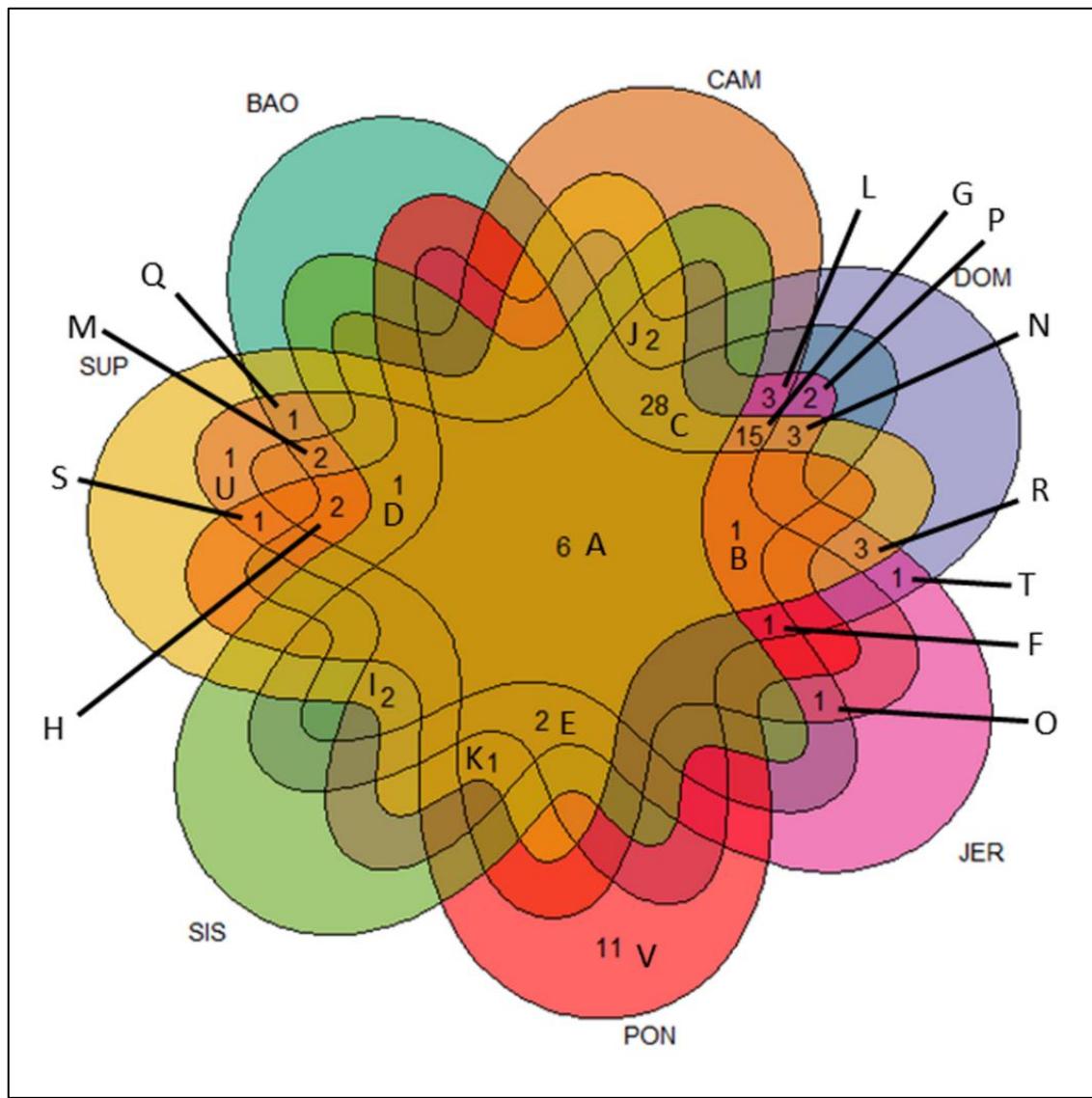
| A – BAO ∪ CAM ∪ DOM ∪ JER ∪ SIS ∪ SUP                    | 6          |
|--|------------|
| Heptanal   |            |
| Anisole  |            |
| 2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl) |            |
| 2,4-Decadienal (E,E)                                     |            |
| 2,4-Decadienal (E,Z)                                     |            |
| Docosane   |            |
| Dodecane   |            |
| Eicosane   |            |
| Farnesol   |            |
| Geraniol   |            |
| Heneicosane  |            |
| Heptacosane  | 35 (44.3%) |
| Heptadecane  |            |
| (E)-2-Heptadecene  |            |
| (E)-3-Heptadecene  |            |
| 7-heptadecene  |            |
| Hexacosane   |            |
| Hexadecanoic acid, methyl ester                          |            |
| 1-Hexadecene   |            |
| 2-Hexadecene   |            |
| Methyl octadecanoate                                     |            |
| 2-Methyl-2-pentenal                                      |            |
| Methyl tetradecanoate                                    |            |
| Octacosane   |            |

|   |             |
|---|-------------|
| Octadecane  |             |
| Octanal   |             |
| Pentacosane   |             |
| 2-Phenyl ethanol  |             |
| Phytane   |             |
| <i>p</i> -Cresol  |             |
| Tetracosane   |             |
| Tricosane   |             |
| 9-Tricosene   |             |
| Tridecane   |             |
| Unidentified_2  |             |
| <b>B - BAO ∪ CAM ∪ DOM ∪ JER ∪ SUP</b>                    | <b>5</b>    |
| β-Caryophyllene   |             |
| <i>cis</i> -Verbenol                                      |             |
| Decanal   |             |
| Decanoic acid   |             |
| g-Terpinene   |             |
| β-Sesquiphellandrene                                      |             |
| 2-Decenal, (E)  |             |
| Dodecanoic acid   | 16 (20.25%) |
| <i>g</i> -eudesmol  |             |
| Hexadecane  |             |
| Linalool  |             |
| 3-Methyloctadecane  |             |
| Pinocarvone   |             |
| Tetradecane   |             |
| <i>trans</i> - β-Farnesene                                |             |
| Unidentified_1  |             |
| <b>C - BAO ∪ CAM ∪ JER ∪ SIS ∪ SUP</b>                    | <b>5</b>    |
| β-Phorone   | 1 (1.26%)   |
| <b>D - BAO ∪ DOM ∪ JER ∪ SIS ∪ SUP</b>                    | <b>5</b>    |
| 1-Octanol   | 1 (1.26%)   |
| <b>E - CAM ∪ DOM ∪ JER ∪ SIS ∪ SUP</b>                    | <b>5</b>    |
| 7,9-di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione |             |
| 1-heptadecene   | 4 (5.06%)   |
| (Z)-3-Heptadecene   |             |
| Hexadecanoic acid   |             |
| <b>F - BAO ∪ CAM ∪ DOM ∪ JER</b>                          | <b>4</b>    |
| Borneol   |             |
| Diacetone alcohol   | 4 (5.06%)   |
| 6-methyl-5-hepten-2-one                                   |             |
| Pentadecane, 2,6,10-trinethyl                             |             |
| <b>G - BAO ∪ CAM ∪ JER ∪ SUP</b>                          | <b>4</b>    |
| α-Phellandren-8-ol  |             |
| Terpinen-4-ol   | 4 (5.06%)   |
| <i>trans</i> -Verbenol                                    |             |
| Verbenone   |             |
| <b>H - BAO ∪ DOM ∪ JER ∪ SUP</b>                          | <b>4</b>    |
| Camphor   |             |
| Decane  | 3 (3.80%)   |
| <i>o</i> -Xylene  |             |

|  |           |
|--|-----------|
| <b>I – CAM <math>\cup</math> JER <math>\cup</math> SIS <math>\cup</math> SUP</b> | <b>4</b>  |
| Nonadecane   | 1 (1.26%) |
| <b>L – BAO <math>\cup</math> CAM <math>\cup</math> JER</b>                       | <b>3</b>  |
| (Z)-2-Heptadecene  | 1 (1.26%) |
| <b>M – BAO <math>\cup</math> DOM <math>\cup</math> JER</b>                       | <b>3</b>  |
| Bornyl acetate   | 2 (2.53%) |
| 4-Methyloctane   |           |
| <b>N – BAO <math>\cup</math> JER <math>\cup</math> SUP</b>                       | <b>3</b>  |
| Nonacosane   | 1 (1.26%) |
| <b>O – DOM <math>\cup</math> JER <math>\cup</math> SUP</b>                       | <b>3</b>  |
| 2-Ethylhexanol   |           |
| 1-Octadecene   | 3 (3.80%) |
| Unidentified_3   |           |
| <b>P – DOM <math>\cup</math> JER</b>   | <b>2</b>  |
| 1-Tetradecene  | 1 (1.26%) |
| <b>Q – JER <math>\cup</math> SUP</b>   | <b>2</b>  |
| $\beta$ -Phellandren-8-ol  | 2 (2.53%) |
| Nonanoic acid  |           |



**Figure S1.** PCA plots of individuals (panel A) and variables (panel B) comprehensive of Ponzone population. In panel A individuals are represented by coloured dots, different colours indicating different geographical origin of the samples, as reported in the legend (BAO= Bau Onu, CAM= Capo Mannu, DOM= Domusnovas, JER= Jerzu, PON= Ponzone, SIS= Sant'Isidoro, SUP= Su Planu). Panel B reports the 44 most contributing variables to the PCA. Variables are represented as arrows originating from the intersection between the two principal axis. Arrows length and colour (from hot to cold colour) are proportional to the contribution of each variable to the PCA. Variables pointing the same direction should be considered as directly proportional, while variables pointing opposite directions should be considered inversely proportional. Variables pointing towards clusters of individuals should be considered highly representative of the features of that cluster.



**Figure S2.** Venn's diagram with the number of compounds shared among Sardinian and Ponzone populations. The letters refer to the supplementary table (Table S3) reporting the identity of the compounds shared by the localities (BAO= Bau Onu, CAM= Capo Mannu, DOM= Domusnovas, JER= Jerzu, PON= Ponzone, SIS= Sant'Isidoro, SUP= Su Planu).

**Table S3.** Integration table to Figure S2. The list of compounds shared by populations (BAO= Bau Onu, CAM= Capo Mannu, DOM= Domusnovas, JER= Jerzu, SIS= Sant'Isidoro, SUP= Su Planu) is reported in the first column. The second column reports the number of populations sharing compounds in each group, the number of compounds shared and the percentage in relation to the total number of compounds identified. The red letter preceding the list of populations refers to the areas in the Venn diagram (Figure S2).

|  |             |
|--|-------------|
| <b>A – BAO ∪ CAM ∪ DOM ∪ JER ∪ PON ∪ SIS ∪ SUP</b>       | 7           |
| 2,4-Decadienal ( <i>E,E</i> )                            |             |
| Heptadecane  |             |
| 1-Hexadecene   |             |
| Pentacosane  | 6 (6.67%)   |
| <i>p</i> -Cresol   |             |
| Tricosane  |             |
| <b>B – BAO ∪ CAM ∪ DOM ∪ JER ∪ PON ∪ SUP</b>             | 6           |
| Decanal  | 1 (1.11%)   |
| <b>C – BAO ∪ CAM ∪ DOM ∪ JER ∪ SIS ∪ SUP</b>             | 6           |
| Anisole  |             |
| 2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl) |             |
| 2,4-Decadienal ( <i>E,Z</i> )                            |             |
| Docosane   |             |
| Dodecane   |             |
| Eicosane   |             |
| Farnesol   |             |
| Geraniol   |             |
| Heneicosane  |             |
| Heptacosane  |             |
| ( <i>E</i> )-2-Heptadecene                               |             |
| ( <i>E</i> )-3-Heptadecene                               |             |
| 7-heptadecene  |             |
| Heptanal   | 28 (38.11%) |
| Hexacosane   |             |
| Hexadecanoic acid, methyl ester                          |             |
| 2-Hexadecene   |             |
| Methyl octadecanoate                                     |             |
| 2-Methyl-2-pentenal                                      |             |
| Methyl tetradecanoate                                    |             |
| Octacosane   |             |
| Octadecane   |             |
| Octanal  |             |
| 2-Phenyl ethanol   |             |
| Phytane  |             |
| Tetracosane  |             |
| 9-Tricosene  |             |
| Tridecane  |             |
| <b>D – BAO ∪ CAM ∪ JER ∪ PON ∪ SIS ∪ SUP</b>             | 6           |
| β-Phorone  | 1 (1.11%)   |
| <b>E – CAM ∪ DOM ∪ JER ∪ PON ∪ SIS ∪ SUP</b>             | 6           |
| 1-heptadecene  | 2 (2.22%)   |
| Hexadecanoic acid  |             |
| <b>F – BAO ∪ CAM ∪ DOM ∪ JER ∪ PON</b>                   | 5           |
| Diacetone alcohol  | 1 (1.11%)   |

|   |             |
|---|-------------|
| <b>G – BAO U CAM U DOM U JER U SUP</b>                    | <b>5</b>    |
| β-Caryophyllene   |             |
| β-Sesquiphellandrene                                      |             |
| <i>cis</i> -Verbenol                                      |             |
| Decanoic acid   |             |
| 2-Decenal, ( <i>E</i> )                                   |             |
| Dodecanoic acid   |             |
| g-eudesmol  |             |
| g-Terpinene   | 15 (16.67%) |
| Hexadecane  |             |
| Linalool  |             |
| 3-Methyloctadecane  |             |
| Pinocarvone   |             |
| Tetradecane   |             |
| <i>trans</i> -b-Farnesene                                 |             |
| Unidentified 1  |             |
| <b>H – BAO U CAM U JER U PON U SUP</b>                    | <b>5</b>    |
| Terpinen-4-ol   |             |
| <i>trans</i> -Verbenol                                    | 2 (2.22%)   |
| <b>I – BAO U DOM U JER U SIS U SUP</b>                    | <b>5</b>    |
| 1-Octanol   |             |
| Unidentified 2  | 2 (2.22%)   |
| <b>J – CAM U DOM U JER U SIS U SUP</b>                    | <b>5</b>    |
| 7,9-di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione |             |
| ( <i>E</i> )-3-Heptadecene                                | 2 (2.22%)   |
| <b>K – CAM U JER U PON U SIS U SUP</b>                    | <b>5</b>    |
| Nonadecane  | 1 (1.11%)   |
| <b>L – BAO U CAM U DOM U JER</b>                          | <b>4</b>    |
| Borneol   |             |
| 6-methyl-5-hepten-2-one                                   | 3 (3.33%)   |
| Pentadecane, 2,6,10-trinethyl                             |             |
| <b>M – BAO U CAM U JER U SUP</b>                          | <b>4</b>    |
| α-Phellandren-8-ol  |             |
| Verbenone   | 2 (2.22%)   |
| <b>N – BAO U DOM U JER U SUP</b>                          | <b>4</b>    |
| Camphor   |             |
| Decane  | 3 (3.33%)   |
| <i>o</i> -Xylene  |             |
| <b>O – BAO U CAM U JER</b>                                | <b>3</b>    |
| ( <i>Z</i> )-2-Heptadecene                                | 1 (1.11%)   |
| <b>P – BAO U DOM U JER</b>                                | <b>3</b>    |
| Bornyl acetate  |             |
| 4-Methyloctane  | 2 (2.22%)   |
| <b>Q – BAO U JER U SUP</b>                                | <b>3</b>    |
| Nonacosane  | 1 (1.11%)   |
| <b>R – DOM U JER U SUP</b>                                | <b>3</b>    |
| 2-Ethylhexanol  |             |
| 1-Octadecene  | 3 (3.33%)   |
| Unidentified 3  |             |
| <b>S – JER U PON U SUP</b>                                | <b>3</b>    |
| Nonanoic acid   | 1 (1.11%)   |

|                        |             |
|------------------------|-------------|
| <b>T - DOM ∪ JER</b>   | <b>2</b>    |
| 1-Octadecene           | 1 (1.11%)   |
| <b>U - JER ∪ SUP</b>   | <b>2</b>    |
| β-Phellandren-8-ol     | 1 (1.11%)   |
| <b>V - PON</b>         | <b>1</b>    |
| α-Isophorone           |             |
| α-Terpineol            |             |
| 2,4 Di-tertbutylphenol |             |
| Heptanoic acid         |             |
| Isopropyl myristate    |             |
| Nonanal                | 11 (12.22%) |
| Octadecanal            |             |
| 2-Phenoxy ethanol      |             |
| <i>p</i> -Cimen-8-ol   |             |
| <i>p</i> -Vinyl-phenol |             |
| Unidentified 5         |             |