Data on free and bound volatile compounds in six *Ribes nigrum* L. blackcurrant cultivars

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**Abstract**

The data investigated 198 volatile compounds of six currant cultivars grown in China which is analyzed by SPME–GC–MS. Volatile compounds in these currant samples were identified by two methods, comparing retention indices with reference standards and matching mass spectrum in the NST11 library. A synthetic currant matrix prepared according to the currant juice condition were extracted and analyzed using the same extraction procedure as the currant samples. The standard curve was generated for quantification of volatile compounds. For the volatiles without the available standard, the data provided consulting standards that had the same carbon atom or the similar functional structure for quantification. Further interpretation and discussion can be seen in article entitled “Characterization of Free and Bound Volatile Compounds in Six *Ribes nigrum* L. Blackcurrant Cultivars” (Liu et al., 2018) [1].

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**Specifications Table**

| Subject area       | Chemistry |
|--------------------|-----------|
| More specific subject area | Aroma |
| Type of data       | Table |
| How data was acquired | GC–MS (Agilent 7890 gas chromatography and an Agilent 5975 mass spectrometer) with automated HS-SPME |
| Data format        | Analyzed |
| Experimental factors | Each currant cultivar was mashed and centrifuge to obtain currant juice. The currant juice was mixed with NaCl and 4-methyl-2-pentanol (internal standard). The bound volatile extraction was released by AR2000 enzyme solution. |
| Experimental features | The free and bound volatile extraction was analyzed by HS-SPME followed by GC–MS using a 60 m × 0.25 mm, 0.25 µm thickness HP-INNOWAX capillary column. |
| Data source location | The horticultural experimental station at the Northeast Agricultural University in China (latitude 44°04′ and longitude 125°42′) |
| Data accessibility | Data is provided with this article. |

**Value of the data**

- This data provided physicochemical parameters of six currant cultivars for further studies of currant quality control.
- Total 198 Volatile compounds were identified in six currant cultivars by GC–MS.
- The standard curve of some volatile compounds was generated for quantification of volatile compounds by GC–MS. The data can be used for reference of volatiles quantification.
- The data calculated the retention indices of volatiles compounds that can be used for qualitative analysis by GC–MS.

1. **Data**

   See Tables 1–3.

2. **Experimental design, materials and methods**

   2.1. **Currant samples**

   Six cultivars of currant (“Risagar”, “Fertodi”, “Brodthrop”, “Sofya”, “Yadrionaya”, and “Liangye”) were obtained from the horticultural experimental station at the Northeast Agricultural University in China (latitude 44°04′ and longitude 125°42′) at their maturity stage. The currant samples were frozen at -20°C prior to further analysis (Table 1).

2.2. **Chemicals and reagents**

   Glucose, sodium hydroxide, sodium chloride, citric acid, and sodium dihydrogen phosphate were obtained from Beijing Chemical Works (Beijing, China). HPLC grade dichloromethane, ethanol, and methanol were purchased from Honeywell (Morris Township, NJ, USA). Pure water was obtained from Milli-Q purification system (Millipore, Bedford, MA, USA). The volatile standards used for identification were purchased from Sigma-Aldrich (St. Louis, MO, USA) with a purity above 98%. Other reagents were of analytical grade unless specifically noted.
2.3. Volatile extraction

Each currant cultivar was mashed and centrifuged to yield currant juice. The currant juice (5 mL) was mixed with NaCl (1.00 g) and 1.0018 g/L 4-methyl-2-pentanol (10 µL, internal standard) in a 15-mL glass vial containing a magnetic stirrer with a PTFE-silicon septum. The mixture was equilibrated on a heating and agitation platform at 40 °C for 30 min. The free volatile compounds in the sample were concentrated with headspace SPME regarding our previous report [2]. Each currant cultivar was conducted in three independent extractions.

The bound volatiles were released using AR2000 enzyme solution according to our published methods [2]. Afterwards, the bound volatile compounds were extracted and analyzed using the same SPME as the free volatile compounds.

2.4. GC–MS analysis

The volatile compounds analysis on GC followed our previous method [3]. An Agilent 7890 gas chromatography equipped with an Agilent 5975 mass spectrometer (Agilent Technologies, Santa Clara, CA, USA) was used to analyze volatile compounds. A 60 m × 0.25 mm, 0.25 µm thickness HP-INNOWAX capillary column (J&W Scientific, Folsom, CA, USA) was used to separate the volatile compounds using the carrier gas (helium) at 1 mL/min flow rate. The over temperature was programmed as follows: 50 °C held for 1 min, then increased from 50 °C to 220 °C at a rate of 3 °C/min and held at 220 °C for 5 min, and then increased to 250 °C at 5 °C/min and held at 250 °C for 5 min. The temperature of MS transfer line was set at 280 °C. Mass spectrum was recorded at 70 eV with 130 °C in the electron impact (EI) mode. All scan mass from m/z 25 to 300 was recorded. C₆-C₂₄ alkane series (Supelco, Bellefonte, PA, USA) was analyzed under the same chromatographic conditions for calculation of retention indices of volatiles. The volatiles in currant were identified by comparing their retention indices and mass spectrum with reference standard. The volatiles without the available standard were tentatively identified by comparing their retention indices and mass spectrum with the NIST11 library (Table 3).

2.5. Standards analysis

A synthetic currant matrix was prepared regarding the physicochemical index of the currant juice. The synthetic currant matrix consisted of 170 g/L sugar and 3.5 g/L citric acid with its pH adjusted 4.0 using 5 M NaOH solution. Each external volatile standard was dissolved in HPLC-grade ethanol to generate the stock standard solution. These stock standard solutions were then combined using the synthetic matrix to form standard working solution. Afterwards, the standards working solution was diluted using the synthetic matrix to 18 successive levels. The standards were analyzed using the same extraction procedure as the currant samples, and analyzed under the same GC method. The standard curve was integrated using the peak area ratio of external volatile standard to internal standard versus the concentration of external standard (Table 2).

### Table 1

| Cultivar | Juice yield (%) | pH | Total soluble solid (°Brix) | Titratable acid (g/L) |
|----------|----------------|----|----------------------------|----------------------|
| Sofya    | 65.07 ± 1.73 b | 2.66 ± 0.01 a | 14.80 ± 0.14 a | 3.34 ± 0.13 ab |
| Yadronaya| 66.36 ± 1.10 b | 2.68 ± 0.01 ab | 15.04 ± 0.00 b | 3.15 ± 0.09 a |
| Liangye  | 53.06 ± 0.64 a | 2.81 ± 0.01 c | 16.15 ± 0.07 c | 4.03 ± 0.04 bc |
| Risagar  | 52.49 ± 1.22 a | 2.68 ± 0.03 ab | 17.25 ± 0.07 d | 4.52 ± 0.21 c |
| Fertodi  | 51.46 ± 2.06 a | 2.65 ± 0.02 a | 18.05 ± 0.21 f | 4.25 ± 0.43 c |
| Brodtrop | 60.45 ± 4.46 ab| 2.74 ± 0.00 b | 15.05 ± 0.21 ab| 3.06 ± 0.04 a |

*a* expressed as citric acid. Data are mean ± standard deviation of triplicate tests. Different letters in each column indicate significant differences at a significant level of 0.05.
| Compounds | CAS no. | Characteristic Ions (m/z) | Quantitative ion (m/z) | Range (μg L⁻¹) | Regression equation | R² |
|-----------|---------|---------------------------|------------------------|----------------|---------------------|----|
| **Alcohols** | | | | Max | Min |
| Heptanol | 111706 | 70,564,355 | 70 | 211.00 | 0.21 | \( y = 1147.1x + 1.4069 \) | 0.976 |
| 1-Octanol | 111875 | 567,084 | 56 | 6.56 | 0.01 | \( y = 7025.9x + 0.1283 \) | 0.991 |
| Isopentanol | 123513 | 55,424,341 | 55 | 1413.80 | 0.69 | \( y = 19779x + 31.211 \) | 0.952 |
| Isohexanol | 626891 | 56,414,342 | 56 | 94.00 | 1.47 | \( y = 5358.2x + 0.8578 \) | 0.990 |
| 2-Heptanol | 543497 | 454,355 | 45 | 51.50 | 0.10 | \( y = 748.37x + 0.2814 \) | 0.994 |
| 1-Hexanol | 111273 | 56,434,155 | 56 | 493.50 | 0.48 | \( y = 1546.3x - 5.0952 \) | 0.885 |
| (Z)-3-Hexen-1-ol | 928961 | 6,741,395,582 | 67 | 2035.00 | 3.97 | \( y = 13,476x + 2.371 \) | 0.990 |
| 3-Octanol | 589980 | 59,558,341 | 59 | 103.13 | 25.78 | \( y = 16,945x + 36.908 \) | 0.914 |
| Benzyl alcohol | 100516 | 79,108,107 | 79 | 1135.00 | 17.73 | \( y = 36,338x + 36.142 \) | 0.994 |
| **Aldehydes** | | | | Max | Min |
| Decanal | 112312 | 4,341,575,544 | 43 | 19.40 | 0.02 | \( y = 2272.1x - 0.2855 \) | 0.962 |
| Hexanal | 66251 | 4,456,414,357 | 44 | 7870.00 | 3.84 | \( y = 7081x - 8.15 \) | 0.988 |
| (E)-2-Hexenal | 6728263 | 41,423,983 | 83 | 40,220.00 | 4.91 | \( y = 11726x - 704.46 \) | 0.982 |
| Nonanal | 124196 | 57,414,356 | 57 | 13.00 | 3.25 | \( y = 648.61x + 1.9932 \) | 0.884 |
| Octanal | 124130 | 4,344,415,684 | 43 | 6.56 | 0.01 | \( y = 70.259x + 0.1283 \) | 0.991 |
| Benzaldehyde | 100527 | 771,061,055,150 | 77 | 58.75 | 0.46 | \( y = 1782x + 1.4342 \) | 0.993 |
| **Acids** | | | | Max | Min |
| Butyric Acid | 107926 | 607,341 | 60 | 120.00 | 15.00 | \( y = 21,865x + 42.766 \) | 0.907 |
| Hexanoic acid | 142621 | 6,073,414,387 | 60 | 104.38 | 26.09 | \( y = 8519.9x + 30.542 \) | 0.781 |
| Heptanoic acid | 111148 | 607,343 | 60 | 580.00 | 9.06 | \( y = 5021.9x + 40.935 \) | 0.952 |
| Octanoic Acid | 124072 | 6,073,434,155 | 60 | 2210.00 | 138.13 | \( y = 35,255x + 219.26 \) | 0.933 |
| **Esters** | | | | Max | Min |
| Ethyl acetate | 141786 | 43 | 43 | 7440.00 | 116.25 | \( y = 7923.88x + 0.0075 \) | 0.999 |
| Ethyl 2-hydroxybenzoate | 118616 | 120 | 120 | 31.50 | 0.25 | \( y = 537.33x + 1.7861 \) | 0.963 |
| Ethyl butanoate | 105344 | 714,329 | 71 | 103.20 | 3.23 | \( y = 1624.7x + 6.7199 \) | 0.976 |
| Isoamyl acetate | 123922 | 43,705,587 | 70 | 202.20 | 1.58 | \( y = 948.91x + 9.6091 \) | 0.953 |
| Ethyl hexanoate | 123660 | 8899 | 88 | 193.60 | 0.38 | \( y = 628.86x + 9.0529 \) | 0.921 |
| Hexyl acetate | 142927 | 435,684 | 84 | 50.30 | 0.20 | \( y = 739.31x + 0.1564 \) | 0.985 |
| Ethyl octanoate | 111115 | 7487 | 74 | 3.00 | 0.38 | \( y = 318.11x + 0.3035 \) | 0.992 |
| Ethyl caprylate | 106321 | 88,127 | 88 | 103.30 | 0.05 | \( y = 1049.9x + 4.7153 \) | 0.945 |
Table 2 (continued)

| Compounds               | CAS no.  | Characteristic Ions (m/z) | Quantitative ion (m/z) | Range (μg L⁻¹) | Regression equation | R²  |
|-------------------------|----------|---------------------------|------------------------|----------------|---------------------|-----|
|                         |          |                           |                        | Max           |                     |     |
|                         |          |                           |                        | Min           |                     |     |
| Terpenoids              |          |                           |                        |               |                     |     |
| Linalool                | 78706    | 71,414,393                | 71                     | 0.15          | 0.00                | 0.996 |
| Neral                   | 106263   | 41                        | 41                     | 0.01          | 0.04                | 0.960 |
| Paracymene              | 99876    | 11,913,491,120            | 119                    | 22.00         | 0.17                | 0.926 |
| Nerol                   | 106252   | 69,419,368                | 69                     | 0.02          | 0.00                | 0.968 |
| Geraniol                | 106241   | 69,41,6829                | 69                     | 0.03          | 0.00                | 0.966 |
| Sulcatone               | 110930   | 43                        | 43                     | 120.00        | 0.12                | 0.993 |
| β-Myrcene               | 123353   | 41,936,939                | 41                     | 0.02          | 0.00                | 0.958 |
| Furan linalool oxide    | 98555    | 5,993,121,136             | 59                     | 0.11          | 0.00                | 0.971 |
| α-Terpineol             |          |                           |                        |               |                     |     |
| (Z)-β-Damascenone       | 23726934 | 121                       | 121                    | 2.27          | 0.28                | 0.995 |
| (E)-β-Damascenone       | 23726934 | 69                        | 69                     | 2.27          | 0.04                | 0.994 |
| Benzene                 |          |                           |                        |               |                     |     |
| Benzaldehyde            | 100527   | 771,061,055,150           | 77                     | 58.75         | 0.46                | 0.993 |
| Methyl 4-hydroxybenzoate| 119368   | 120,152                   | 120                    | 69.00         | 0.54                | 0.910 |
| 2-Phenyethanol          | 60128    | 91,122                    | 91                     | 649.38        | 5.07                | 0.995 |
| Phenol                  | 108952   | 946,665                   | 94                     | 43.40         | 0.01                | 0.979 |
| p-Ethylguaiacol         | 2785899  | 137,152                   | 137                    | 39.60         | 0.62                | 0.960 |
| p-Ethylphenol           | 123079   | 107,122                   | 107                    | 6.23          | 0.39                | 0.976 |
| Styrene                 | 100425   | 104,103,787,751           | 104                    | 129.00        | 1.01                | 0.960 |
| NO. | NO. | Compound                        | RI   | Quantitative analysis | Quantification m/z | Quantitative standard curve | Classification   |
|-----|-----|---------------------------------|------|-----------------------|---------------------|----------------------------|------------------|
| 1   | A1  | Acetic acid                     | 1449 | RI, Mass              | 60                  | Butyric Acid Acids          |                  |
| 2   | A2  | Propionic Acid                  | 1534 | RI, Mass              | 74                  | Butyric Acid Acids          |                  |
| 3   | A3  | Isobutyric acid                 | 1563 | RI, Mass              | 43                  | Butyric Acid Acids          |                  |
| 4   | A4  | Pivalic acid                    | 1573 | RI, Mass              | 57                  | Ethyl caprylate Acids       |                  |
| 5   | A5  | Butyric Acid                    | 1622 | Str, RI, Mass         | 60                  | Butyric Acid Acids          |                  |
| 6   | A6  | Isovaleric acid                 | 1664 | RI, Mass              | 60                  | Butyric Acid Acids          |                  |
| 7   | A7  | 2-Ethylbutanoic acid            | 1665 | RI, Mass              | 74                  | Butyric Acid Acids          |                  |
| 8   | A8  | Valeric acid                    | 1732 | RI, Mass              | 60                  | Hexanoic acid Acids         |                  |
| 9   | A9  | Hexanoic acid                   | 1840 | Str, RI, Mass         | 60                  | Hexanoic acid Acids         |                  |
| 10  | A10 | 2-Ethylhexanoic acid            | 1944 | RI, Mass              | 73                  | Hexanoic acid Acids         |                  |
| 11  | A11 | Heptanoic acid                  | 1947 | Str, RI, Mass         | 60                  | Heptanoic acid Acids        |                  |
| 12  | A12 | Octanoic Acid                   | 2052 | Str, RI, Mass         | 60                  | Octanoic Acid Acids         |                  |
| 13  | A13 | Nonanoic acid                   | 2155 | RI, Mass              | 60                  | Octanoic Acid Acids         |                  |
| 14  | L14 | Hexanal                         | 1041 | Str, RI, Mass         | 56                  | Hexanal Aldehyde            |                  |
| 15  | L15 | (E)-2-Hexenal                   | 1220 | Str, RI, Mass         | 41                  | (E)-2-Hexenal Aldehyde     |                  |
| 16  | L16 | Octanal                         | 1280 | Str, RI, Mass         | 43                  | Octanal Aldehyde            |                  |
| 17  | L17 | (E)-2-Heptenal                  | 1323 | RI, Mass              | 41                  | Hexanal Aldehyde            |                  |
| 18  | L18 | Nonanal                         | 1385 | Str, RI, Mass         | 57                  | Nonanal Aldehyde            |                  |
| 19  | L19 | 1-Formyl-5-ethylcyclopentene    | 1414 | RI, Mass              | 124                 | Decanal Aldehyde            |                  |
| 20  | L20 | (E)-2-Octenal                   | 1428 | RI, Mass              | 41                  | Decanal Aldehyde            |                  |
| 21  | L21 | Decanal                         | 1492 | Str, RI, Mass         | 43                  | Decanal Aldehyde            |                  |
| 22  | L22 | Benzaldehyde                     | 1523 | Str, RI, Mass         | 77                  | Benzaldehyde Aldehyde       |                  |
| 23  | -   | p-Tolualdehyde                  | 1650 | RI, Mass              | 91                  | Benzaldehyde Aldehyde       |                  |
| 24  | L24 | 2-Isopropenyl-5-methylhex-4-enal | 1684 | Mass                  | 69                  | Decanal Aldehyde            |                  |
| 25  | L25 | (E,E)-2,4-Nonadienal            | 1703 | RI, Mass              | 81                  | Decanal Aldehyde            |                  |
| 26  | L26 | Cuminaldehyde                   | 1785 | RI, Mass              | 133                 | Benzaldehyde Aldehyde       |                  |
| 27  | L27 | 3,4-Dimethylbenzaldehyde        | 1818 | RI, Mass              | 133                 | Benzaldehyde Aldehyde       |                  |
| 28  | B28 | Styrene                         | 1232 | Str, RI, Mass         | 104                 | Styrene Benzene             |                  |
| 29  | B29 | 2,5-Dimethylstyrone             | 1429 | RI, Mass              | 117                 | Benzylalcohol Benzene       |                  |
| 30  | B30 | p-Cymene                        | 1411 | RI, Mass              | 117                 | Benzylalcohol Benzene       |                  |
| 31  | B31 | 2,4-Dimethylstyrone             | 1415 | RI, Mass              | 117                 | Benzylalcohol Benzene       |                  |
| 32  | B32 | 2-Allyltoluene                  | 1420 | RI, Mass              | 117                 | Benzylalcohol Benzene       |                  |
| 33  | B33 | Hypnon                          | 1651 | RI, Mass              | 105                 | Benzaldehyde Benzene        |                  |
| 34  | B34 | Veratrol                        | 1704 | RI, Mass              | 138                 | p-Ethylguaicacol Benzene    |                  |
| 35  | B35 | 3-Hydroxy-3-phenylbutan-2-one   | 1750 | Mass                  | 43                  | 2-Phenyethanol Benzene      |                  |
| 36  | B36 | Methyl 4-hydroxybenzoate        | 1777 | Str, RI, Mass         | 120                 | Methyl 4-hydroxybenzoate    |                  |
| 37  | B37 | 2-Methylanthalene               | 1857 | RI, Mass              | 142                 | Benzylalcohol Benzene       |                  |
| NO. | NO.a | Compound                      | RI     | Quantitative analysis\(^b\) | Quantification \(m/z\) | Quantitative standard curve\(^d\) | Classification       |
|-----|------|-------------------------------|--------|-----------------------------|------------------------|----------------------------------|----------------------|
| 38  | B38  | 1-Methylnaphthalene           | 1891   | R.I., Mass 142               | Benzylic alcohol       | Benzene                          |
| 39  | B39  | Butylhydroxytoluene           | 1913   | R.I., Mass 205               | Benzaldehyde           | Benzene                          |
| 40  | B40  | 1,2-Benzisothiazole           | 1959   | R.I., Mass 135               | Benzylic alcohol       | Benzene                          |
| 41  | B41  | 5-Hydroxyindan                | 2481   | Mass 133                     | \(p\)-Ethylphenol      | Benzene                          |
| 42  | B42  | Guaiacol                      | 1859   | Str, R.I., Mass 109          | Guaiacol               | Volatile Phenols                 |
| 43  | B43  | \(o\)-Cresol                  | 1998   | R.I., Mass 108               | \(p\)-Ethylphenol      | Volatile Phenols                 |
| 44  | B44  | Phenol                        | 2001   | Str, R.I., Mass 94           | Phenol                 | Volatile Phenols                 |
| 45  | B45  | \(p\)-Ethylguaiacol           | 2027   | Str, R.I., Mass 137          | \(p\)-Ethylguaiacol   | Volatile Phenols                 |
| 46  | B46  | 2,5-Xylenol                   | 2072   | R.I., Mass 122               | \(p\)-Ethylphenol      | Volatile Phenols                 |
| 47  | B47  | \(p\)-Cresol                  | 2077   | R.I., Mass 107               | \(p\)-Ethylphenol      | Volatile Phenols                 |
| 48  | –    | Eugenol                       | 2160   | R.I., Mass 164               | \(p\)-Ethylphenol      | Volatile Phenols                 |
| 49  | B49  | \(p\)-Ethylphenol             | 2165   | Str, R.I., Mass 107          | \(p\)-Ethylphenol      | Volatile Phenols                 |
| 50  | B50  | 4-Vinylguaiacol               | 2187   | R.I., Mass 150               | \(p\)-Ethylguaiacol   | Volatile Phenols                 |
| 51  | B51  | 2,4-Di-tert-butylphenol       | 2289   | R.I., Mass 191               | \(p\)-Ethylphenol      | Volatile Phenols                 |
| 52  | B52  | 4-Formyl-2,6-di-tert-butylphenol | 2461 | Mass 219 | \(p\)-Ethylphenol | Volatile Phenols                  |
| 53  | E53  | Isoamyl acetate               | 1114   | Str, R.I., Mass 43           | Isoamyl acetate        | Acetate Esters                   |
| 54  | E54  | Hexyl acetate                 | 1261   | Str, R.I., Mass 43           | Hexyl acetate          | Acetate Esters                   |
| 55  | E55  | \((Z)-3\)-Hexenol acetate    | 1308   | R.I., Mass 43                | Ethyl hexanoate        | Acetate Esters                   |
| 56  | E56  | \((E)-2\)-Hexenol acetate    | 1324   | R.I., Mass 43                | Ethyl hexanoate        | Acetate Esters                   |
| 57  | E57  | Furfuryl acetate              | 1530   | R.I., Mass 43                | Ethyl caprylate        | Acetate Esters                   |
| 58  | E58  | Bornyl acetate                | 1576   | R.I., Mass 95                | Ethyl caprylate        | Acetate Esters                   |
| 59  | E59  | Benzyl acetate                | 1727   | R.I., Mass 108               | Ethyl 2-hydroxybenzoate | Acetate Esters                   |
| 60  | E60  | 2-Phenetyl acetate            | 1816   | R.I., Mass 104               | Ethyl 2-hydroxybenzoate | Acetate Esters                   |
| 61  | E61  | Ethyl acetate                 | 691    | Str, R.I., Mass 43           | Ethyl acetate          | Ethyl esters                     |
| 62  | E62  | Ethyl butanoate               | 899    | Str, R.I., Mass 71           | Ethyl butanoate        | Ethyl esters                     |
| 63  | E63  | Ethyl hexanoate               | 1222   | Str, R.I., Mass 88           | Ethyl hexanoate        | Ethyl esters                     |
| 64  | E64  | Ethyl octanoate               | 1387   | Str, R.I., Mass 74           | Ethyl octanoate        | Ethyl esters                     |
| 65  | E65  | Ethyl 2-hydroxybutanoate      | 1403   | R.I., Mass 59                | Ethyl 2-hydroxybenzoate | Ethyl esters                     |
| 66  | E66  | Ethyl caprylate               | 1425   | Str, R.I., Mass 88           | Ethyl caprylate        | Ethyl esters                     |
| 67  | E67  | Ethyl 3-hydroxybutyrate       | 1516   | R.I., Mass 43                | Ethyl 2-hydroxybenzoate | Ethyl esters                     |
| 68  | E68  | Ethyl benzoate                | 1666   | R.I., Mass 105               | Ethyl 2-hydroxybenzoate | Ethyl esters                     |
| 69  | E69  | Ethyl 3-hydroxyhexanoate      | 1677   | R.I., Mass 71                | Ethyl 2-hydroxybenzoate | Ethyl esters                     |
| 70  | E70  | Ethyl 2-hydroxybenzoate       | 1813   | Str, R.I., Mass 120          | Ethyl 2-hydroxybenzoate | Ethyl esters                     |
| 71  | E71  | Methyl butanoate              | 785    | R.I., Mass 74                | Ethyl butanoate        | Other Esters                     |
| 72  | E72  | Methyl caproate               | 1186   | R.I., Mass 74                | Ethyl butanoate        | Other Esters                     |
| 73  | E73  | Butyl butanoate               | 1207   | R.I., Mass 71                | Ethyl butanoate        | Other Esters                     |
| 74  | E74  | Methyl 2-hydroxybutyrate      | 1379   | R.I., Mass 59                | Ethyl 2-hydroxybenzoate | Other Esters                     |
| 75  | E75  | Methyl 3-hydroxybutyrate      | 1478   | Mass 43                      | Ethyl 2-hydroxybenzoate | Other Esters                     |
| No. | Code | Name of Compound | RI | Mass | Code | Name of Compound | RI | Mass |
|-----|------|------------------|----|------|------|------------------|----|------|
| 76  | E76  | Methyl 2-hydroxy-3-methylpentanoate | 1490 | RI, Mass | 90  | Ethyl 2-hydroxybenzoate | Other Esters |
| 77  | E77  | Methyl 2-hydroxyhexanoate | 1575 | RI, Mass | 69  | Ethyl 2-hydroxybenzoate | Other Esters |
| 78  | E78  | Methyl decanoate | 1590 | RI, Mass | 74  | Ethyl caprylate | Other Esters |
| 79  | E79  | Methyl benzoate | 1620 | RI, Mass | 105 | Ethyl 2-hydroxybenzoate | Other Esters |
| 80  | E80  | Methyl 3-hydroxypropionate | 1645 | RI, Mass | 43  | Ethyl 2-hydroxybenzoate | Other Esters |
| 81  | E81  | Methyl 2-hydroxyoctanoate | 1784 | Mass | 97  | Ethyl caprylate | Other Esters |
| 82  | E82  | 3-Hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate | 1869 | RI, Mass | 71  | Ethyl caprylate | Other Esters |
| 83  | E83  | 2,4,4-trimethyl-1,3-pentanediyl bis(2-methylpropanoate) | 1880 | Mass | 71  | Ethyl caprylate | Other Esters |
| 84  | E84  | 1-hydroxy-2,4,4-trimethyl-3-pentanyl 2-methylpropanoate | 1885 | Mass | 71  | Ethyl caprylate | Other Esters |
| 85  | E85  | Methyl 5-methylsalicylate | 1902 | Mass | 134 | Ethyl 2-hydroxybenzoate | Other Esters |
| 86  | E86  | Diisobutyl glutarate | 2008 | Mass | 115 | Ethyl caprylate | Other Esters |
| 87  | E87  | 2-Isooctoxyethyl benzoate | 2128 | Mass | 105 | Ethyl 2-hydroxybenzoate | Other Esters |
| 88  | H88  | 2-Pentanol | 1135 | RI, Mass | 45  | 2-Heptanol | Higher Alcohols |
| 89  | H89  | Isopentanol | 1214 | Str, RI, Mass | 55  | Isopentanol | Higher Alcohols |
| 90  | H90  | Pentyl alcohol | 1253 | RI, Mass | 42  | 1-Hexanol | Higher Alcohols |
| 91  | H91  | 3-Heptanol | 1291 | RI, Mass | 59  | 2-Heptanol | Higher Alcohols |
| 92  | H92  | 2-Methyl-1-pentanol | 1297 | RI, Mass | 43  | Isopentanol | Higher Alcohols |
| 93  | H93  | 4-Pentenol | 1299 | RI, Mass | 67  | (E)-2-Hexene-1-ol | Higher Alcohols |
| 94  | H94  | (E)-2-Penten-1-ol | 1309 | RI, Mass | 57  | (E)-2-Hexene-1-ol | Higher Alcohols |
| 95  | H95  | Isohexanol | 1310 | Str, RI, Mass | 56  | Isohexanol | Higher Alcohols |
| 96  | H96  | 2-Heptanol | 1315 | Str, RI, Mass | 45  | 2-Heptanol | Higher Alcohols |
| 97  | H97  | 3-Methylpentanol | 1323 | RI, Mass | 56  | Isohexanol | Higher Alcohols |
| 98  | H98  | 1-Hexanol | 1349 | Str, RI, Mass | 56  | 1-Hexanol | Higher Alcohols |
| 99  | H99  | 4-Methyl-2-heptanol | 1353 | Mass | 45  | Isohexanol | Higher Alcohols |
| 100 | H100 | 6-Methyl-2-heptanol | 1368 | RI, Mass | 45  | Isohexanol | Higher Alcohols |
| 101 | H101 | (Z)-3-Hexen-1-ol | 1381 | Str, RI, Mass | 67  | (Z)-3-Hexen-1-ol | Higher Alcohols |
| 102 | H102 | 4-Methyl-3-pentenol | 1384 | RI, Mass | 41  | Isohexanol | Higher Alcohols |
| 103 | H103 | 3-Octanol | 1387 | Str, RI, Mass | 59  | 3-Octanol | Higher Alcohols |
| 104 | H104 | (E)-2-Hexene-1-ol | 1401 | Str, RI, Mass | 57  | (E)-2-Hexene-1-ol | Higher Alcohols |
| 105 | H105 | 4-Methylhexanol | 1424 | RI, Mass | 70  | 1-Octanol | Higher Alcohols |
| 106 | H106 | Heptanol | 1448 | Str, RI, Mass | 70  | Heptanol | Higher Alcohols |
| 107 | H107 | 1-Octanol | 1551 | Str, RI, Mass | 56  | 1-Octanol | Higher Alcohols |
| 108 | H108 | Norbornyl alcohol | 1561 | Mass | 94  | 1-Octanol | Higher Alcohols |
| 109 | H109 | (E)-2-Octen-1-ol | 1609 | RI, Mass | 57  | (E)-2-Hexene-1-ol | Higher Alcohols |
| 110 | H110 | (Z)-5-Octen-1-ol | 1609 | RI, Mass | 67  | (E)-2-Hexene-1-ol | Higher Alcohols |
| 111 | H111 | 1-Nonanol | 1654 | RI, Mass | 56  | 1-Octanol | Higher Alcohols |
| 112 | H112 | (Z)-3-Nonen-1-ol | 1679 | RI, Mass | 81  | (E)-2-Hexene-1-ol | Higher Alcohols |
| 113 | H113 | 2-Hydroxyoctene | 1756 | RI, Mass | 43  | 2-Phenylethanol | Higher Alcohols |
| 114 | H114 | Decanol | 1758 | RI, Mass | 70  | 1-Octanol | Higher Alcohols |
| 115 | H115 | p-Phenylethanol | 1810 | RI, Mass | 79  | Benzylalcohol | Higher Alcohols |
| 116 | H116 | p-Cymene-8-ol | 1847 | RI, Mass | 43  | 2-Phenylethanol | Higher Alcohols |
| NO. | Compound                        | RI    | Quantitative analysis | Quantification m/z | Quantitative standard curve | Classification          |
|-----|---------------------------------|-------|-----------------------|--------------------|-----------------------------|-------------------------|
| 117 | H117 Benzylalcohol              | 1875  | Str, RI, Mass         | 79                 | Benzyalcohol                | Higher Alcohols         |
| 118 | H118 2-Phenylethanol            | 1911  | Str, RI, Mass         | 91                 | 2-Phenylethanol             | Higher Alcohols         |
| 119 | H119 2,4-Dimethylphenethyl alcohol | 2017 | Mass                  | 119                | 2-Phenylethanol             | Higher Alcohols         |
| 120 | H120 p-Isopropylbenzyl alcohol  | 2098  | RI, Mass              | 135                | 2-Phenylethanol             | Higher Alcohols         |
| 121 | K121 2-Octanone                 | 1281  | RI, Mass              | 43                 | Decanal                     | Ketones                 |
| 122 | K122 Acetoin                    | 1297  | RI, Mass              | 45                 | 1-Hexanol                   | Ketones                 |
| 123 | K123 2,3-Octanediene            | 1315  | RI, Mass              | 43                 | Decanal                     | Ketones                 |
| 124 | K124 Tyranton                   | 1367  | RI, Mass              | 43                 | Ethyl hexanoate             | Ketones                 |
| 125 | K125 3-Methyl-3-cyclohexen-1-one| 1411  | Mass                  | 67                 | Decanal                     | Ketones                 |
| 126 | K126 (E,E)-3,5-Octadien-2-one   | 1569  | RI, Mass              | 95                 | Decanal                     | Ketones                 |
| 127 | K127 2-Furyl ethyl ketone       | 1634  | RI, Mass              | 81                 | Decanal                     | Ketones                 |
| 128 | K128 Sabina ketone              | 1674  | RI, Mass              | 96                 | Styrene                     | Ketones                 |
| 129 | K129 Cryptone                   | 1373  | RI, Mass              | 126                | Styrene                     | Others                  |
| 130 | O130 Dimethyl trisulfide        | 1706  | RI, Mass              | 85                 | Styrene                     | Others                  |
| 131 | O131 Tonkalide                  | 1720  | RI, Mass              | 41                 | Styrene                     | Others                  |
| 132 | O132 2-Methyl-2-butenolide      | 1973  | RI, Mass              | 99                 | Ethyl 3-hydroxybutanoate    | Others                  |
| 133 | O133 5-Octanolide               | 2361  | RI, Mass              | 20                 | Benzy alcohol               | Others                  |
| 134 | – Coumaran                      | 1456  | RI, Mass              | 95                 | Ethyl caprylate             | Norisoprenoids          |
| 135 | T135 6-Methyl-5-hepten-2-ol     | 934   | RI, Mass              | 71                 | –                           | Terpenoids              |
| 136 | – Vinylidimethylcarbinol        | 1127  | RI, Mass              | 93                 | Terpinolen                  | Terpenoids              |
| 137 | T137 3-Karen                    | 1139  | RI, Mass              | 93                 | Terpinolen                  | Terpenoids              |
| 138 | T138 Nopinen                    | 1142  | RI, Mass              | 93                 | Terpinolen                  | Terpenoids              |
| 139 | T139 Menthaadiene               | 1156  | RI, Mass              | 93                 | Terpinolen                  | Terpenoids              |
| 140 | T140 Terpilene                  | 1187  | RI, Mass              | 93                 | Terpinolen                  | Terpenoids              |
| 141 | T141 α-Phellandrene             | 1199  | RI, Mass              | 43                 | Terpinolen                  | Terpenoids              |
| 142 | T142 Cineole                    | 1226  | RI, Mass              | 93                 | Terpinolen                  | Terpenoids              |
| 143 | T143 Cithemene                  | 1253  | Str, RI, Mass         | 119                | Paracymene                  | Terpenoids              |
| 144 | T144 Paracymene                 | 1265  | RI, Mass              | 93                 | Terpinolen                  | Terpenoids              |
| 145 | T145 Terpinolene                | 1321  | RI, Mass              | 71                 | –                           | Terpenoids              |
| 146 | – Prenol                        | 1333  | Str, RI, Mass         | 43                 | Sulfatone                   | Terpenoids              |
| 147 | T147 Sulcatone                  | 1356  | RI, Mass              | 139                | Furan linalool oxide        | Terpenoids              |
| 148 | T148 Rosoxide                   | 1360  | Mass                  | 121                | β-Myrcene                   | Terpenoids              |
| 149 | T149 3,4-Dimethyl-2,4,6-octatriene| 1441 | RI, Mass              | 59                 | Furan linalool oxide        | Terpenoids              |
| 150 | T150 cis-Linalooloxide          | 1469  | Mass                  | 59                 | Furan linalool oxide        | Terpenoids              |
| 151 | T151 Linalol oxide A            | 1516  | RI, Mass              | 95                 | α-Terpineol                 | Terpenoids              |
| 152 | T152 Camphor                    | 1520  | RI, Mass              | 121                | Terpinolen                  | Terpenoids              |
| No. | Compound Name                                      | RI, Mass   | Mass  | α-Terpineol Terpenoids |
|-----|---------------------------------------------------|------------|-------|------------------------|
| 154 | 1,4-Dimethyl-4-acetylcyclohexene                   | 1541       | 109   |                        |
| 155 | Linalool                                           | 1591       | 94    |                        |
| 156 | L-4-terpineol                                      | 1592       | 92    |                        |
| 157 | Caryophyllene                                      | 1614       | 94    |                        |
| 158 | p-Mentha-1-en-9-ol                                | 1637       | 71    |                        |
| 159 | Menthol                                           | 1653       | 92    |                        |
| 160 | Pinocarveol                                       | 1656       | 43    |                        |
| 161 | Cepheine                                          | 1658       | 139   |                        |
| 162 | 2,2,3-Trimethyl-3-cyclopentene-1-ethanol          | 1660       | 43    |                        |
| 163 | Borneol                                           | 1668       | 95    |                        |
| 164 | Phellandral                                       | 1704       | 109   |                        |
| 165 | 6-[(2-Hydroxy-2-propyl)-3-methyl-2-cyclohexen-1-yl acetate | 1715       | 59    |                        |
| 166 | 6-Methyl-2-vinyl-5-hepten-1-ol                    | 1726       | 41    |                        |
| 167 | 2-Hydroxycineol                                   | 1726       | 108   |                        |
| 168 | Lilac alcohol formate A                           | 1731       | 55    |                        |
| 169 | Piperitone                                         | 1731       | 82    |                        |
| 170 | Neral                                             | 1733       | 41    |                        |
| 171 | Carvone                                           | 1736       | 82    |                        |
| 172 | Linalool oxide                                    | 1736       | 68    |                        |
| 173 | Lilac alcohol B                                   | 1743       | 55    |                        |
| 174 | cis-p-Menth-2-en-7-ol                             | 1753       | 93    |                        |
| 175 | L-Verbenone                                       | 1754       | 107   |                        |
| 176 | (Z)-α-Damascenone                                 | 1760       | 121   |                        |
| 177 | D-Citronellol                                     | 1761       | 41    |                        |
| 178 | 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-2-buten-1-one | 1744       | 121   | β-Ionone              |
| 179 | trans-p-Menth-2-en-7-ol                           | 1772       | 93    |                        |
| 180 | 1,7,7-Trimethylbicyclo[2.2.1] hept-5-en-2-ol       | 1776       | 108   |                        |
| 181 | 7-Methyl-3-methylene-6-octen-1-ol                 | 1782       | 69    |                        |
| 182 | Lilac alcohol C                                   | 1786       | 55    |                        |
| 183 | Perillal                                          | 1789       | 68    |                        |
| 184 | Nerol                                             | 1796       | 69    |                        |
| 185 | Isogeraniol                                       | 1808       | 41    |                        |
| 186 | (E)-α-Damascenone                                 | 1822       | 69    |                        |
| 187 | 2-Hydroxycineol                                   | 1827       | 55    |                        |
| 188 | Lilac alcohol D                                   | 1833       | 109   |                        |
| 189 | (Z)-Carveol                                       | 1843       | 69    |                        |
| 190 | Geraniol                                          | 1858       | 108   |                        |
| 191 | p-Menth-1-en-9-ol                                 | 1937       | 94    |                        |
| 192 | p-Menth-1,4-dien-7-ol                             | 1946       | 79    |                        |
| NO. | NO. | Compound                  | RI      | Quantitative analysis | Quantification m/z | Quantitative standard curve | Classification |
|-----|-----|---------------------------|---------|-----------------------|--------------------|-----------------------------|----------------|
| 194 | T194| Perilla alcohol           | 1993    | RI, Mass              | 68                 | α-Terpineol                 | Terpenoids      |
| 195 | T195| p-Menthadien-7-ol         | 2087    | Mass                  | 79                 | α-Terpineol                 | Terpenoids      |
| 196 | T196| Spathulenol               | 2123    | Mass                  | 43                 | α-Terpineol                 | Terpenoids      |
| 197 | T197| 7-epi-α-selinene          | 2166    | Mass                  | 161                | Terpinolene                 | Terpenoids      |
| 198 | T198| Bisabolol                 | 2207    | RI, Mass              | 43                 | α-Terpineol                 | Terpenoids      |

* Numbers of compounds used for principal component analysis in article entitled “Characterization of Free and Bound Volatile Compounds in Six Ribes nigrum L. Blackcurrant Cultivars” [1].

* Quantitative Analysis – Str: identified with standard substance; RI: RI agreed with database of NIST11; Mass: mass spectrum agreed with the mass spectral database.

* Quantification m/z – the main fragment of compound for quantification.

* Quantitative Standard Curve – the compound was quantified by the standard curve of compounds with similar structure.
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Transparency document. Supplementary material

Transparency data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2018.01.090.

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