

**Table S1.** Headspace volatile compounds of cili wines fermented by different yeasts.

|                 |                       |            |          |         |                | Yeast Strain   |              |                           |              |              |              |              |              |              |              |
|-----------------|-----------------------|------------|----------|---------|----------------|----------------|--------------|---------------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| No              | Compounds             | CAS        | RI Calc. | RI Lit. | Identification | X16            | S103         | S102                      | F33          | GV107        | SH12         | RMS2         | CZ           | Prelude      | Pre-CZ       |
|                 |                       |            |          |         |                | Content (mg/L) |              |                           |              |              |              |              |              |              |              |
| Higher alcohols |                       |            |          |         |                |                |              |                           |              |              |              |              |              |              |              |
| 1               | 1-Propanol            | 71-23-8    | 1031     | 1044    | RI, MS         | 0.50±0.05a     | nd           | 0.48±0.07a                | nd           | nd           | nd           | 0.74±0.05b   | 0.41±0.06a   | nd           | 0.67±0.06b   |
| 2               | 2-Methyl-1-propanol   | 78-83-1    | 1093     | 1092    | RI, MS         | 4.06±0.80a     | 4.23±0.09a   | 2.88±0.42b                | 1.82±0.18c   | 3.10±0.43b   | 2.47±0.23c   | 2.60±0.65bc  | 3.34±0.22b   | 1.31±0.03d   | 3.18±0.48b   |
| 3               | 1-Penten-3-ol         | 616-25-1   | 1153     | 1158    | RI, MS         | nd             | nd           | nd                        | nd           | nd           | nd           | nd           | nd           | 0.22±0.03    | nd           |
| 4               | 1-Butanol             | 71-36-3    | 1139     | 1136    | RI, MS         | nd             | nd           | nd                        | 12.23±3.25a  | 0.15±0.01a   | nd           | nd           | nd           | nd           | nd           |
| 5               | 3-Methyl-1-butanol    | 123-51-3   | 1203     | 1209    | RI, MS         | 108.05±12.98a  | 102.75±2.67a | 92.26±14.51b <sub>c</sub> | 65.36±11.94c | 97.21±3.45ab | 69.85±6.22d  | 91.48±14.85c | 76.87±9.19c  | 79.17±10.05c | 77.88±11.74c |
| 6               | 1-Pentanol            | 71-41-0    | 1243     | 1252    | RI, MS         | 0.26±0.04b     | 0.33±0.10a   | 0.23±0.05c                | 0.17±0.06d   | 0.23±0.04c   | 0.30±0.08a   | 0.25±0.02b   | 0.19±0.04cd  | 0.26±0.06b   | 0.25±0.05b   |
| 7               | Hexyl alcohol         | 111-27-3   | 1343     | 1359    | RI, MS         | 2.59±0.29a     | 2.33±0.15b   | 2.48±0.43ab               | 1.30±0.30d   | 2.75±0.16a   | 2.44±0.24b   | 2.43±0.47b   | 2.29±0.24b   | 1.62±0.32c   | 2.53±0.46a   |
| 8               | (E)-3-Hexen-1-ol      | 928-97-2   | 1355     | 1352    | RI, MS         | nd             | nd           | nd                        | nd           | 0.57±0.09b   | nd           | nd           | nd           | nd           | 0.83±0.12a   |
| 9               | 3-Ethoxy-1-propanol   | 111-35-3   | 1368     | 1359    | RI, MS         | nd             | nd           | nd                        | nd           | nd           | nd           | nd           | nd           | 0.18±0.02    | nd           |
| 10              | Leaf alcohol          | 928-96-1   | 1376     | 1371    | RI, MS         | 27.31±3.38ab   | 25.66±0.58b  | 26.02±4.07b               | 16.60±3.54d  | 27.56±1.62a  | 25.39±2.33b  | 25.98±4.08b  | 23.66±3.09c  | 22.44±2.96c  | 27.13±4.15ab |
| 11              | (R, R)-2,3-Butanediol | 24347-58-8 | 1531     | 1544    | RI, MS         | 2.44±0.60ab    | 1.65±0.53d   | 2.00±0.14c                | 3.09±0.73a   | 2.99±1.53a   | 2.04±0.80c   | 2.83±0.19b   | 1.89±0.25d   | 2.53±0.88b   | 2.11±0.51c   |
| 12              | 2-Nonanol             | 628-99-9   | 1507     | 1525    | RI, MS         | nd             | nd           | nd                        | nd           | nd           | 0.50±0.05    | nd           | nd           | nd           | nd           |
| 13              | 1-Octanol             | 111-87-5   | 1547     | 1546    | RI, MS         | 0.48±0.05b     | nd           | nd                        | nd           | nd           | nd           | nd           | 0.50±0.03b   | 0.15±0.01c   | 0.88±0.14a   |
| 14              | Furfuryl alcohol      | 98-00-0    | 1654     | 1665    | RI, MS         | nd             | nd           | nd                        | nd           | nd           | 0.43±0.14    | nd           | nd           | nd           | nd           |
| 15              | Phenethyl alcohol     | 60-12-8    | 1906     | 1912    | RI, MS         | nd             | 13.80±0.78c  | 17.24±2.43b               | 29.03±6.14a  | 17.93±1.89b  | 13.81±0.78   | 18.82±0.65b  | 11.58±1.68c  | 18.03±3.85b  | 13.78±4.78c  |
| 16              | Decyl alcohol         | 112-30-1   | 1749     | 1752    | RI, MS         | nd             | nd           | nd                        | nd           | nd           | nd           | nd           | nd           | nd           | 0.83±0.28    |
| Σ               |                       |            |          |         |                | 145.69±22.68   | 150.76±4.91  | 143.57±22.13              | 117.61±22.97 | 152.49±9.23  | 177.23±10.88 | 145.04±20.98 | 120.73±14.81 | 125.91±18.19 | 130.08±22.78 |
| Acids           |                       |            |          |         |                |                |              |                           |              |              |              |              |              |              |              |
| 17              | Acetic acid           | 64-19-7    | 1444     | 1449    | RI, MS         | 3.85±0.41ab    | 3.14±0.42b   | 3.36±0.71b                | 1.02±0.56d   | 3.05±10.8b   | 3.49±0.831b  | 3.13±0.79b   | 3.14±0.13b   | 2.15±0.67c   | 4.21±0.61a   |
| 18              | Octanoic acid         | 124-07-2   | 2045     | 2050    | RI, MS         | 21.53±0.64d    | 19.76±0.28f  | 20.89±4.32e               | 34.19±14.65c | 17.26±3.64f  | 20.03±2.36d  | 23.40±2.07e  | 27.73±8.10d  | 38.24±5.07ab | 40.14±2.55a  |
| 19              | Decanoic acid         | 334-48-5   | 2258     | 2275    | RI, MS         | 0.82±0.19g     | 0.87±0.07g   | 2.58±0.80d                | 16.78±1.23a  | 2.27±0.23d   | 3.18±0.89c   | 2.06±1.09d   | 1.71±0.11f   | 7.37±2.29b   | 3.82±0.82c   |

|    |                               |            |      |      |        |              |             |               |               |              |               |               |               |              |                |
|----|-------------------------------|------------|------|------|--------|--------------|-------------|---------------|---------------|--------------|---------------|---------------|---------------|--------------|----------------|
| 20 | 9-Decenoic acid               | 14436-32-9 | 2320 | 2341 | RI, MS | 1.21±0.16g   | nd          | 2.38±0.85d    | nd            | nd           | 1.85±0.12f    | 2.67±1.21c    | 3.42±0.67bc   | 6.13±1.97a   | 3.83±0.89b     |
| 21 | (E)-3-Hexenoic acid           | 1577-18-0  | 1944 | NA   | MS     | nd           | nd          | nd            | nd            | nd           | nd            | nd            | nd            | 0.11±0.01    | nd             |
|    | $\Sigma$                      |            |      |      |        | 27.39±1.39   | 23.77±0.77  | 29.22±6.68    | 51.99±16.44   | 22.58±4.96   | 34.55±4.20    | 31.28±5.16    | 36.01±9.01    | 54.00±9.34   | 52.00±4.87     |
|    | <i>Esters</i>                 |            |      |      |        |              |             |               |               |              |               |               |               |              |                |
| 22 | Ethyl acetate                 | 141-78-6   | 879  | 891  | RI, MS | 11.46±1.55b  | 12.46±0.84b | 10.94±1.46bc  | 7.28±1.19d    | 9.08±0.40c   | 11.90±1.20b   | 10.74±1.59bc  | 11.06±1.25b   | 25.53±2.52a  | 14.00±2.22b    |
| 23 | Isobutyl acetate              | 110-19-0   | 1007 | 1007 | RI, MS | 0.19±0.04d   | nd          | nd            | 0.19±0.02d    | nd           | nd            | nd            | 0.33±0.04c    | 0.76±0.14a   | 0.43±0.05b     |
| 24 | Ethyl propionate              | 105-37-3   | 951  | 951  | MS     | nd           | nd          | nd            | nd            | nd           | nd            | nd            | nd            | 0.47±0.11    | nd             |
| 25 | n-Propyl acetate              | 109-60-4   | 967  | 968  | RI, MS | nd           | nd          | nd            | nd            | nd           | nd            | nd            | nd            | 1.51±0.57    | nd             |
| 26 | Ethyl butyrate                | 105-54-4   | 1029 | 1025 | RI, MS | 1.19±0.18e   | 1.89±0.34d  | 2.05±0.27c    | 1.28±0.16e    | 1.86±0.20d   | 2.30±0.23bc   | 1.86±0.43d    | 2.02±0.22c    | 3.81±0.34a   | 2.61±0.38b     |
| 27 | 2-Pentylacetate               | 626-38-0   | 1063 | 1074 | RI, MS | nd           | nd          | nd            | nd            | nd           | nd            | nd            | nd            | 0.08±0.02    | nd             |
| 28 | Isoamyl acetate               | 123-92-2   | 1115 | 1112 | RI, MS | 24.11±5.27c  | 32.12±4.30b | 18.79±2.93d   | 17.46±2.79d   | 19.30±1.03d  | 18.43±1.87d   | 15.07±6.09f   | 25.79±3.00c   | 78.08±6.24a  | 39.01±7.18b    |
| 29 | cis-2-Pentenyl acetate        | 42125-10-0 | 1216 | NA   | MS     | nd           | nd          | nd            | nd            | nd           | 0.19±0.04b    | nd            | nd            | 0.14±0.01c   | 0.27±0.04a     |
| 30 | Ethyl hexanoate               | 123-66-0   | 1224 | 1228 | RI, MS | 23.86±3.40f  | 24.47±3.70f | 38.21±5.90d   | 36.36±5.78d   | 41.30±2.08c  | 43.65±3.99c   | 51.13±5.54ab  | 46.23±6.10b   | 69.90±10.04a | 64.05±10.60a   |
| 31 | Hexyl acetate                 | 142-92-7   | 1263 | 1279 | RI, MS | 3.10±0.47f   | 3.13±0.62f  | 2.75±0.43g    | 1.96±1.21h    | 2.56±0.35g   | 4.15±0.52d    | 3.01±0.61f    | 5.66±0.63c    | 9.63±1.55a   | 7.69±1.21b     |
| 32 | (E)-3-Hexenyl acetate         | 3681-82-1  | 1311 | 1306 | RI, MS | 26.65±4.08c  | 26.95±2.46c | 21.05±3.27d   | 16.09±2.94e   | 20.50±1.56d  | 23.34±1.96d   | 20.20±3.91d   | 29.19±2.36c   | 50.78±4.92a  | 44.88±7.06b    |
| 33 | Ethyl octanoate               | 106-32-1   | 1427 | 1435 | RI, MS | 74.96±14.22d | 56.87±5.82d | 130.87±18.63c | 159.34±20.20b | 125.99±9.79c | 123.11±11.69c | 208.67±49.49a | 152.00±16.28b | 205.53±2.95a | 187.39±44.67ab |
| 34 | Ethyl 2-furoate               | 614-99-3   | 1619 | 1611 | RI, MS | nd           | nd          | 0.40±0.10a    | nd            | nd           | 0.41±0.06a    | nd            | 0.40±0.08a    | 0.34±0.09b   | nd             |
| 35 | 1,2-Dimethylethylene acetate  | 1114-92-7  | 1479 | 1484 | RI, MS | 0.69±0.37b   | nd          | nd            | nd            | nd           | 0.93±0.82a    | nd            | nd            | 0.59±0.04c   | nd             |
| 36 | (Z)-Ethyl pentadec-9-enoate   | 56219-09-1 | 1885 | NA   | MS     | nd           | nd          | nd            | nd            | nd           | nd            | nd            | nd            | 2.20±0.23    | nd             |
| 37 | 3-Octenoic acid, pentyl ester | 55656-58-1 | 1520 | NA   | MS     | nd           | nd          | nd            | nd            | nd           | nd            | nd            | nd            | 0.30±0.06    | nd             |
| 38 | Ethyl trans-2-Octenoate       | 7367-82-0  | 1547 | NA   | MS     | nd           | nd          | nd            | nd            | nd           | 0.80±0.21     | nd            | nd            | nd           | nd             |
| 39 | Ethyl decanoate               | 110-38-3   | 1628 | 1648 | RI, MS | 5.02±1.26f   | 4.77±0.53f  | 17.84±8.71d   | 65.87±12.20a  | 13.54±1.89e  | 17.06±5.25d   | 25.20±1.02bc  | 17.85±5.75d   | 34.65±9.43b  | 19.41±3.56d    |
| 40 | 3-methylbutyl octanoate       | 2035-99-6  | 1648 | 1670 | RI, MS | 0.94±0.62b   | 0.65±0.17d  | 0.36±0.07f    | 0.59±0.13d    | 0.45±0.08f   | 0.57±0.11d    | 0.70±0.26c    | 0.77±0.14bc   | 1.83±0.42a   | nd             |
| 41 | Ethyl 9-decenoate             | 67233-91-4 | 1682 | 1703 | RI, MS | 22.65±4.32f  | 15.73±2.13g | 33.20±7.60d   | 7.50±3.89h    | 21.99±2.39f  | 25.80±2.20e   | 39.00±0.93c   | 61.61±5.18b   | 87.07±8.60a  | 56.27±11.62b   |

|                        |                            |            |      |                    |               |              |              |              |              |              |              |              |              |              |              |
|------------------------|----------------------------|------------|------|--------------------|---------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| 42                     | Phenethyl acetate          | 103-45-7   | 1812 | 1847               | <i>RI, MS</i> | 3.71±0.33bc  | 3.31±0.18c   | 2.44±0.78e   | 7.07±1.53a   | 2.52±0.21d   | 1.87±0.18f   | 3.16±0.04c   | 2.81±0.33d   | 8.08±0.96a   | 4.37±0.66b   |
| 43                     | Isoamyl decanoate          | 2306-91-4  | 1851 | 1653. <sub>4</sub> | <i>RI, MS</i> | nd           | nd           | nd           | 0.46±0.04a   | nd           | nd           | 0.31±0.02b   | 0.40±0.15ab  | 0.47±0.09a   | nd           |
| 44                     | Ethyl myristate            | 124-06-1   | 2036 | 1799. <sub>4</sub> | <i>RI, MS</i> | nd           | 0.29±0.04e   | 1.30±0.93a   | 0.84±0.09bc  | 0.68±0.06d   | 0.61±0.09d   | 0.68±0.17d   | 1.04±0.14a   | 0.89±0.05b   | nd           |
| 45                     | Ethyl laurate              | 106-33-2   | 1832 | 1593               | <i>RI, MS</i> | nd           | nd           | 11.53±3.41b  | 21.01±2.93a  | 9.18±0.96c   | nd           | 11.41±2.99b  | 12.93±1.00b  | 20.78±0.62a  | 18.78±2.67a  |
| 46                     | Phenethyl propionate       | 122-70-3   | 1879 | NA                 | <i>RI, MS</i> | nd           | nd           | nd           | nd           | nd           | nd           | nd           | nd           | 0.19±0.03    | nd           |
| 47                     | Ethyl palmitate            | 628-97-7   | 2241 | 1993. <sub>5</sub> | <i>RI, MS</i> | nd           | nd           | nd           | 0.36±0.06    | nd           | nd           | nd           | nd           | nd           | nd           |
| $\Sigma$               |                            |            |      |                    |               | 198.50±36.10 | 182.64±21.12 | 291.73±54.49 | 343.64±55.17 | 268.95±21.00 | 275.13±30.42 | 391.14±73.09 | 370.11±42.68 | 603.60±50.02 | 459.14±91.92 |
| <i>Aldehydes</i>       |                            |            |      |                    |               |              |              |              |              |              |              |              |              |              |              |
| 48                     | Acetaldehyde               | 75-07-0    | 697  | 692                | <i>RI, MS</i> | 1.05±0.11c   | 0.94±0.16cd  | 0.70±0.37d   | 1.18±0.08c   | 1.43±0.95c   | 0.94±0.16cd  | 0.86±0.34cd  | 2.14±0.29b   | 0.12±0.01e   | 2.53±0.41a   |
| 49                     | 2,4-Dimethylbenzaldehyde   | 15764-16-6 | 1818 | 1190               | <i>RI, MS</i> | 0.73±0.24b   | 0.72±0.13b   | 0.38±0.05d   | 0.33±0.08e   | nd           | 0.38±0.07d   | nd           | nd           | 0.40±0.05c   | 1.50±0.14a   |
| $\Sigma$               |                            |            |      |                    |               | 1.77±0.35    | 1.66±0.29    | 1.08±0.42    | 1.52±0.16    | 1.43±0.95    | 1.32±0.23    | 0.86±0.33    | 2.14±0.29    | 0.52±0.06    | 4.03±0.55    |
| <i>Phenols</i>         |                            |            |      |                    |               |              |              |              |              |              |              |              |              |              |              |
| 50                     | Butylated hydroxytoluene   | 128-37-0   | 1902 | 1909               | <i>RI, MS</i> | 0.92±0.11e   | 0.64±0.21f   | 1.70±1.31d   | 0.70±0.21f   | nd           | 0.64±0.21f   | 17.66±1.62b  | 12.27±0.19c  | 1.45±0.09d   | 20.45±7.52a  |
| 51                     | 1,2-xylene                 | 95-47-6    | 1130 | 1180               | <i>RI, MS</i> | nd           | nd           | nd           | nd           | 0.17±0.03a   | nd           | nd           | nd           | 0.13±0.05b   | nd           |
| 52                     | Naphthalene                | 91-20-3    | 1745 | 1743               | <i>RI, MS</i> | nd           | nd           | nd           | nd           | nd           | nd           | nd           | nd           | 0.08±0.03    | nd           |
| 53                     | 3,4-Dimethoxystyrene       | 6380-23-0  | 2030 | NA                 | <i>MS</i>     | nd           | nd           | nd           | nd           | nd           | 0.50±0.08    | nd           | nd           | nd           | nd           |
| 54                     | 4-Hydroxy-3-methoxystyrene | 7786-61-0  | 2194 | 2213               | <i>RI, MS</i> | nd           | nd           | nd           | nd           | nd           | 0.37±0.15    | nd           | nd           | nd           | nd           |
| 55                     | 4-Methoxystyrene           | 637-69-4   | 1677 | NA                 | <i>MS</i>     | nd           | nd           | nd           | nd           | nd           | 0.81±0.06    | nd           | nd           | nd           | nd           |
| 56                     | Methyl eugenol             | 93-15-2    | 2145 | NA                 | <i>MS</i>     | nd           | nd           | nd           | nd           | nd           | nd           | nd           | nd           | 0.15±0.02    | nd           |
| 57                     | 2-Ethoxynaphthalene        | 93-18-5    | 2145 | NA                 | <i>RI, MS</i> | nd           | nd           | nd           | 0.66±0.08b   | nd           | nd           | nd           | nd           | 0.35±0.21c   | 1.08±0.22a   |
| $\Sigma$               |                            |            |      |                    |               | 0.92±0.11    | 0.64±0.21    | 1.70±1.31    | 1.36±0.29    | 0.17±0.03    | 2.31±0.49    | 17.66±1.62   | 12.27±0.19   | 2.17±0.39    | 21.54±7.15   |
| <i>Other compounds</i> |                            |            |      |                    |               |              |              |              |              |              |              |              |              |              |              |
| 58                     | DL-Alanyl-L-Alanine        | 59247-16-4 | 798  | NA                 | <i>RI, MS</i> | nd           | nd           | nd           | 9.32±1.45a   | nd           | nd           | nd           | nd           | 5.02±0.24b   | nd           |
| 59                     | 2,3-Dihydrobenzofuran      | 496-16-2   | 2389 | NA                 | <i>RI, MS</i> | nd           | nd           | 0.54±0.13b   | 1.13±0.39a   | nd           | nd           | nd           | nd           | nd           | nd           |

|                      |                   |          |      |      |        |       |       |           |            |            |            |       |       |           |       |
|----------------------|-------------------|----------|------|------|--------|-------|-------|-----------|------------|------------|------------|-------|-------|-----------|-------|
| 60                   | Cyclooctatetraene | 629-20-9 | 1252 | 1264 | RI, MS | nd    | nd    | nd        | 2.03±0.29a | nd         | 1.41±0.12b | nd    | nd    | nd        | nd    |
| 61                   | Dibenzofuran      | 132-64-9 | 2274 | NA   | RI, MS | nd    | nd    | nd        | 0.53±0.05a | 6.95±2.58b | nd         | nd    | nd    | nd        | nd    |
|                      | $\Sigma$          |          |      |      |        | 0     | 0     | 0.54±0.13 | 13.00±2.18 | 6.95±2.58  | 1.41±0.12  | 0     | 0     | 5.02±0.24 | 0     |
| Compounds identified |                   |          |      |      |        | 28    | 25    | 29        | 33         | 31         | 36         | 29    | 31    | 46        | 33    |
| Total identified (%) |                   |          |      |      |        | 70.00 | 54.35 | 59.20     | 58.90      | 59.60      | 60.00      | 61.70 | 56.40 | 67.65     | 59.56 |
| Higher alcohols (%)  |                   |          |      |      |        | 28.57 | 28.00 | 27.59     | 24.24      | 29.03      | 25.00      | 27.59 | 29.03 | 21.74     | 33.33 |
| Acids (%)            |                   |          |      |      |        | 14.29 | 12.00 | 13.79     | 9.09       | 9.68       | 11.11      | 13.79 | 12.90 | 10.87     | 12.12 |
| Esters (%)           |                   |          |      |      |        | 46.43 | 48.00 | 48.28     | 48.48      | 41.94      | 44.44      | 48.28 | 51.61 | 52.17     | 39.39 |
| Aldehydes (%)        |                   |          |      |      |        | 7.14  | 8.00  | 6.90      | 6.06       | 3.23       | 5.56       | 3.45  | 3.23  | 4.35      | 6.06  |
| Volatile phenols (%) |                   |          |      |      |        | 3.57  | 4.00  | 3.45      | 6.06       | 3.23       | 11.11      | 3.45  | 3.23  | 10.87     | 6.06  |
| Others (%)           |                   |          |      |      |        | 0     | 0     | 0         | 6.06       | 12.90      | 2.78       | 3.45  | 0     | 0         | 3.03  |

ßNote: Different letters in the same line show significant differences between samples at the 95% confidence level. The data represent the means of the three replicates from each ferment. Reference indices (RIs) were obtained from the “NIST Chemistry WebBook” (<https://webbook.nist.gov/chemistry/>). \*NA indicates that the reference index was not available. \*nd indicates that the substance was not detected.