Table S1

List of aroma components with observed and model derived odor threshold property

| Sl. No. | NAME                      | observed odor threshold property (log (OT)) | Predicted odor threshold property |
|---------|---------------------------|--------------------------------------------|-----------------------------------|
| 1*      | 1-propanol                | 5.920                                      | 6.198                             |
| 2       | isopropyl alcohol         | 6.397                                      | 6.231                             |
| 3       | isobutyl alcohol          | 5.732                                      | 5.804                             |
| 4       | 1-butanol                 | 6.306                                      | 5.778                             |
| 5*      | isopentyl alcohol         | 5.532                                      | 5.374                             |
| 6       | isohexyl alcohol          | 4.690                                      | 4.950                             |
| 7       | 3-methyl-pentan-1-ol      | 5.167                                      | 4.962                             |
| 8*      | 1-heptanol                | 3.935                                      | 4.446                             |
| 9       | 2-ethyl-1-hexanol         | 4.584                                      | 4.078                             |
| 10      | 1-octanol                 | 3.839                                      | 3.992                             |
| 11      | 2,3-butanediol            | 6.124                                      | 6.038                             |
| 12      | 1-decanol                 | 3.403                                      | 3.976                             |
| 13*     | dodecan-1-ol              | 4.730                                      | 4.658                             |
| 14      | ethyl acetate             | 4.930                                      | 4.386                             |
| 15      | isobutyl acetate          | 4.139                                      | 3.518                             |
| 16      | ethyl butanoate           | 2.236                                      | 2.851                             |
| 17*     | ethyl isovalerate         | 1.362                                      | 2.131                             |
| 18      | isopentyl acetate         | 2.362                                      | 2.900                             |
| 19      | hexyl acetate             | 4.017                                      | 2.707                             |
| 20*     | ethyl hexanoate           | 1.987                                      | 2.109                             |
| 21      | ethyl 2-hydroxy-3-methylbutyrate | 3.534                  | 3.976                             |
| 22      | ethyl octanoate           | 1.463                                      | 2.612                             |
| 23      | ethyl decanoate           | 2.999                                      | 2.296                             |
| 24      | ethyl 9-decenoate         | 2.703                                      | 2.852                             |
| 25      | isopentyl octanoate       | 2.766                                      | 2.666                             |
| 26*     | propanoic acid            | 5.039                                      | 4.730                             |
| 27*     | isobutyric acid           | 4.417                                      | 4.317                             |
| 28      | butyric acid              | 3.285                                      | 4.291                             |
| 29      | isopentanoic acid         | 2.468                                      | 3.881                             |
| 30*     | hexanoic acid             | 3.558                                      | 3.343                             |
| 31      | octanoic acid             | 3.540                                      | 2.984                             |
| 32      | decanoic acid             | 3.764                                      | 2.984                             |
| 33      | 9-decenoic acid           | 3.769                                      | 2.170                             |
| 34      | dodecanoic acid           | 3.698                                      | 3.666                             |
| 35      | (E)-3-hexen-1-ol          | 3.601                                      | 3.275                             |
| 36*     | (Z)-3-hexen-1-ol          | 3.601                                      | 3.300                             |
|   |          |       |       |
|---|----------|-------|-------|
| 37 | linalool  | 2.210 | 2.348 |
| 38 | ALPHA-terpineol | 3.210 | 3.193 |
| 39 | citronellol | 2.806 | 3.162 |
| 40*| trans-geraniol | 2.289 | 2.348 |
| 41 | BETA-ionone | -0.330 | -0.046 |
| 42*| ALPHA-ionone | -0.330 | -0.410 |
| 43 | Beta-damascenone | -0.580 | -1.178 |
| 44 | furfural | 5.167 | 4.056 |
| 45 | furaneol | 4.158 | 4.825 |
| 46 | furfuryl alcohol | 1.591 | 2.186 |
| 48 | 3-hydroxy-4,5-dimethylfuran-2(5H)-one | -0.381 | -0.531 |
| 49*| 3-sulfanylhexanol | -0.350 | -0.302 |
| 50 | 3-sulfanylheptanal | -0.262 | -0.774 |
| 52 | Gama-nonlactone | 2.283 | 2.247 |
| 53*| phenyl acetic acid | 3.866 | 2.984 |
| 54 | 2-phenyl-ethanol | 4.992 | 4.385 |
| 55*| phenethyl acetate | 3.183 | 2.984 |
| 56*| ethyl phenylacetate | 3.597 | 2.984 |
| 57 | methyl salicylate | 3.517 | 2.984 |
| 58 | ethyl 4-hydroxybenzoate | 3.478 | 2.984 |
| 59 | vanillin | 3.119 | 2.984 |
| 60 | ethyl vanillin | 3.775 | 2.984 |
| 61 | eugenol | 1.563 | 2.170 |
| 62 | guaiacol | 1.906 | 3.206 |
| 63 | thymol | 4.221 | 3.094 |
| 64 | alpha-Terpineol | 2.853 | 3.221 |
| 65*| Nerol | 1.988 | 2.348 |
| 66 | cis,trans-Farnesol | 3.653 | 3.239 |
| 67 | Methanol | 7.319 | 6.964 |
| 68 | isoamyl alcohol | 5.532 | 5.374 |
| 69 | 1-Octen-3-ol | 0.892 | 3.162 |
| 70 | Ethyl propanoate | 4.246 | 3.552 |
| 71 | Ethyl butyrate | 2.236 | 2.909 |
| 72 | Ethyl dodecanoate | 3.340 | 3.113 |
| 73 | Ethyl tetradecanoate | 3.892 | 4.054 |
|   |    |                |      |    |
|---|---|----------------|-----|---|
| 74* | Ethyl hexadecanoate | 3.722 | 4.683 |
| 75* | Ethyl isobutyrate    | 2.111 | 2.010 |
| 76  | Ethyl 2-methylbutyrate | 0.885 | 1.430 |
| 77* | Isoamyl acetate      | 2.362 | 2.683 |
| 78  | 2-Phenylethyl acetate | 3.183 | 2.984 |
| 79  | Isoamyl octanoate    | 2.766 | 2.666 |
| 80  | Acetaldehyde         | 5.356 | 5.779 |
| 81  | Benzaldehyde         | 3.275 | 4.088 |
| 82  | Benzyl alcohol       | 6.267 | 4.823 |
| 83  | Ethyl cinnamate      | 0.754 | 1.356 |
| 84* | Ethyl 2-furoate      | 3.853 | 2.984 |
| 85  | Phenol, 4-ethenyl-2-methoxy- | 1.300 | 2.170 |

*denoted test set compounds

**Table S2**

Weightage of descriptors for first two components.

| Descriptors                      | Weightage based on the first two components |
|----------------------------------|---------------------------------------------|
|                                  | Component 1      | Component 2      |
| nR=Cs                            | -0.358618        | -0.332316        |
| O-056                            | 0.318237         | 0.111099         |
| F10[C-C]                         | 0.00186353       | 0.596138         |
| ETA dAlpha                       | -0.376946        | -0.787048        |
| <0.030684-Jurs-FPSA-3>           | -0.257966        | 0.0107757        |
| <128.127-MW>                     | 0.550793         | -0.0489371       |
| <298.581-Jurs-DPSA-2>            | 0.508043         | -0.145935        |
**Table S3**
The steps involved in the calculation of “composite” value of each descriptor.

| Sl no | OT (nmol) | Fraction | Des 1*fraction | Des n*fraction |
|-------|-----------|----------|----------------|----------------|
| 1     | P1        | P1/W1    | d1*(P1/W1)     | dn*(P1/W1)     |
| 2     | P2        | P2/W1    | d1*(P2/W1)     | dn*(P2/W1)     |
|       |           |          |                | n               |
| n     | Pn        | Pn/W1    | d1*(Pn/W1)     | dn*(Pn/W1)     |

Sum=W1

| Sum= composite value of | Sum= composite value of |
|-------------------------|-------------------------|
| descriptor 1            | descriptor n            |

**Table S4**
Results of the “composite” odor threshold property of different wines obtained from the PLS model.

| Types of wine | DW | SW | NR1 | NR2 |
|---------------|----|----|-----|-----|
| Log(OT)       | 5.169 | 4.819 | 4.580 | 4.566 |
Fig. S1. The randomization plot for the QSPR model derived from PLS analysis.
Fig. S2. Regression coefficient plot of the final PLS model.
Fig. S3. Variable importance plot (VIP) for the final PLS model.
Fig. S4. DModX values of the training set compounds at 99% significance level for the developed model. The dash horizontal line signifies the critical DModX value (2.222) at the 99% confidence level.
Fig. S5. DModX values of the test set compounds at 99% significance level for the developed model. The dash horizontal line signifies the critical DModX value (2.222) at the 99% confidence level.
Fig. S6. PCA score plot for selected 20 training set compounds (10 of which have the lowest odor threshold property and 10 of which have the highest odor threshold property) using the model descriptors.