

**Application of metabolomics method in the study of pear fruit storage**  
**Appendix**

| Table 1 Time Group Differential Metabolites |         |         |                     |      |               |
|---------------------------------------------|---------|---------|---------------------|------|---------------|
| Name                                        | Rt(min) | P Value | Log <sub>2</sub> FC | VIP  | Formula       |
| Benzoic acid                                | 21.23   | 0.00    | -7.08               | 1.05 | C18H19NO4     |
| Asparagine                                  | 12.12   | 0.00    | -3.78               | 1.31 | C13H32N2O3Si3 |
| L-Aspartic acid                             | 14.49   | 0.27    | -3.59               | 1.21 | C4 H7 N O4    |
| Succinic semialdehyde                       | 11.90   | 0.00    | -3.56               | 1.16 | C8H17NO3Si    |
| 3-Oxaluric acid                             | 13.57   | 0.01    | -3.42               | 1.04 | C3H4N2O4      |
| Octadecanamide                              | 15.29   | 0.00    | -3.37               | 1.08 | C22H44N2O2    |
| l-Alanine                                   | 17.25   | 0.03    | -3.34               | 1.15 | C21H30F3NO3   |
| Glucosamine hydrochloride                   | 11.25   | 0.00    | -3.29               | 1.12 | C6H13NO5      |
| 1-Pyrroline-2-carboxylate                   | 11.25   | 0.01    | -2.93               | 1.06 | C8H15NO2Si    |
| carboxylic acid, ethyl ester                | 21.16   | 0.01    | -2.75               | 1.13 | C6H8N2O2      |
| Glycine                                     | 11.02   | 0.01    | -2.69               | 1.04 | C11H29NO2Si3  |
| Formamide                                   | 5.60    | 0.02    | -2.30               | 1.07 | CH3NO         |
| Hexane                                      | 6.46    | 0.01    | -2.18               | 1.24 | C18H36        |
| L-Asparagine                                | 11.41   | 0.00    | -2.17               | 1.12 | C10H24N2O3Si2 |
| Nopaline                                    | 11.36   | 0.01    | -2.12               | 1.03 | C11H20N4O6    |
| Propionaldehyde                             | 15.36   | 0.05    | -2.09               | 1.06 | C3H6O         |
| Leucocyanidin                               | 12.37   | 0.00    | -2.07               | 1.03 | C15H14O7      |
| Putrescine                                  | 13.52   | 0.01    | -1.99               | 1.02 | C13H36N2Si3   |
| Aspartic acid                               | 20.37   | 0.01    | -1.79               | 1.02 | C16H39NO4Si4  |
| Hydroxyurea                                 | 11.03   | 0.04    | -1.66               | 1.08 | CH4N2O2       |
| Butanoic acid                               | 19.33   | 0.00    | -1.58               | 1.23 | C13H32O4Si3   |
| Pimelic acid                                | 14.09   | 0.03    | -1.54               | 1.00 | C7H14N2O4     |
| Acetoacetic acid                            | 13.06   | 0.03    | -1.52               | 1.01 | C4H6O3        |
| D-Fructose                                  | 14.06   | 0.01    | 1.04                | 1.06 | C22H55NO6Si5  |
| Methylamine                                 | 21.83   | 0.00    | 1.55                | 1.05 | CH5N.ClH      |
| 1-Phenylethylamine                          | 11.86   | 0.02    | 1.58                | 1.17 | C12H9F6NO2    |
| phenylenediamine                            | 21.23   | 0.00    | 1.70                | 1.28 | C26H20N2      |
| d-Glucose                                   | 14.77   | 0.03    | 1.74                | 1.01 | C22H55NO6Si5  |
| Sarcosine                                   | 11.94   | 0.00    | 1.77                | 1.28 | C9H23NO2Si2   |
| Bisphenol A                                 | 15.86   | 0.03    | 1.78                | 1.17 | C18H24O2Si    |
| Creatinine                                  | 22.02   | 0.18    | 1.83                | 1.16 | C4H7N3O       |
| Cyclohexane                                 | 15.90   | 0.00    | 1.86                | 1.10 | C18H36        |
| Aminohippuric acid                          | 9.69    | 0.03    | 1.99                | 1.24 | C15H24N2O3Si  |
| Creatinine                                  | 16.07   | 0.02    | 2.04                | 1.14 | C10H23N3OSi2  |
| 5-methoxypsoralen                           | 19.09   | 0.03    | 2.09                | 1.16 | C12H8O4       |
| Panthenol                                   | 26.30   | 0.02    | 2.34                | 1.05 | C9H19NO4      |
| Palmitic Acid                               | 16.01   | 0.09    | 2.35                | 1.02 | C19H40O2Si    |
| Tromethamine                                | 11.85   | 0.02    | 2.90                | 1.14 | C16H43NO3Si4  |
| indolepyruvic acid                          | 13.16   | 0.37    | 4.19                | 1.13 | C11H9NO3      |

|                      |      |      |       |      |                 |
|----------------------|------|------|-------|------|-----------------|
| L-Glutamine          | 0.95 | 0.36 | 1.76  | 1.02 | C10 H10 N4 O2 S |
| hexopyranoside       | 1.34 | 0.01 | -1.48 | 1.44 | C25 H28 O11     |
| L-Phenylalanine      | 5.03 | 0.00 | 2.30  | 1.14 | C9 H11 N O2     |
| D-(+)-Maltose        | 1.31 | 0.02 | -0.36 | 1.49 | C12 H22 O11     |
| phthalate            | 1.15 | 0.00 | 1.46  | 1.23 | C17 H16 Cl N3 O |
| Isoleucine           | 3.31 | 0.00 | 2.34  | 1.09 | C6 H13 N O2     |
| L-(-)-Methionine     | 2.47 | 0.00 | 2.01  | 1.21 | C5 H11 N O2 S   |
| Prolylleucine        | 1.97 | 0.00 | 1.50  | 1.27 | C5 H11 N O2 S   |
| thioadenosine        | 5.26 | 0.01 | 1.40  | 1.01 | C11H15N5O3S     |
| carboxylic acid      | 5.77 | 0.00 | 1.65  | 1.12 | C19H24N2O5      |
| octadecadienoic acid | 9.54 | 0.04 | 1.37  | 1.20 | C18 H30 O3      |

Table 2 Differential Metabolites in Temperature Groups

| Name                    | Rt(min) | P Value | Log <sub>2</sub> FC | VIP  | Formula            |
|-------------------------|---------|---------|---------------------|------|--------------------|
| Succinic semialdehyde   | 15.32   | 0.00    | -7.90               | 1.29 | C8H17NO3Si         |
| 10-hydroxydecanoic acid | 15.35   | 0.00    | -4.54               | 1.02 | C10H20O3           |
| Maleamic acid           | 16.33   | 0.00    | -3.64               | 1.09 | C12H25NO3Si2       |
| Octylamine              | 15.89   | 0.00    | -3.63               | 1.01 | C8H19N             |
| Octanoic acid           | 12.36   | 0.00    | -3.62               | 1.04 | C11H24O2Si         |
| 2-hydroxybenzyl alcohol | 15.95   | 0.00    | -3.31               | 1.14 | C7H8O2             |
| Gallic acid             | 9.12    | 0.00    | -2.99               | 1.02 | C7H6O5             |
| 2-Naphthoic acid        | 20.87   | 0.00    | -2.50               | 1.12 | C11H8O4            |
| Phosphonic acid         | 15.95   | 0.00    | -2.39               | 1.09 | C8H19O3P           |
| Propane-1,3-diol        | 23.59   | 0.00    | -2.36               | 1.10 | C13H34O3Si3        |
| Putrescine              | 13.52   | 0.01    | -1.87               | 1.02 | C13H36N2Si3        |
| Methionine              | 19.35   | 0.00    | -1.78               | 1.13 | C5 H11 N O2 S      |
| Spermidine              | 16.38   | 0.00    | -1.65               | 1.11 | C19H51N3Si4        |
| propionic acid          | 15.81   | 0.00    | -1.61               | 1.12 | C3H6O2             |
| beta-Chamigrene         | 21.95   | 0.00    | -1.57               | 1.20 | C15H24             |
| Tetradecanoic acid      | 19.35   | 0.00    | -1.44               | 1.15 | C3(C13)14H36O2Si   |
| Aspartic acid           | 20.37   | 0.01    | -1.43               | 1.07 | C16H39NO4Si4       |
| pyruvic acid            | 10.70   | 0.00    | -1.40               | 1.12 | C11H9NO3           |
| Phosphonic acid         | 10.98   | 0.05    | -1.35               | 1.13 | C7H21O3PSi2        |
| 2-Aminocaprylic acid    | 14.19   | 0.04    | -1.33               | 1.02 | C15H29NO5          |
| Asparagine              | 12.03   | 0.03    | -1.29               | 1.05 | C13H32N2O3Si3      |
| Sinapic acid            | 16.45   | 0.03    | -1.28               | 1.08 | C17H28O5Si2        |
| Thiabendazole           | 13.62   | 0.01    | -1.21               | 1.10 | C10H7N3S           |
| Progesterone            | 13.44   | 0.05    | -1.17               | 1.12 | C21H30O3           |
| D-Glucose 6-phosphate   | 22.02   | 0.02    | -1.16               | 1.28 | C6H11Na2O9P · xH2O |
| Aspartic acid           | 13.62   | 0.04    | -1.13               | 1.08 | C16H39NO4Si4       |
| Naringenin              | 13.51   | 0.01    | -1.12               | 1.06 | C15H12O5           |
| Pentadecanoic acid      | 15.24   | 0.02    | -1.10               | 1.06 | C18H38O2Si         |
| D-Arabinose 5-phosphate | 13.43   | 0.03    | -1.09               | 1.14 | C5H11O8P.Na        |

|                        |       |      |       |      |                  |
|------------------------|-------|------|-------|------|------------------|
| d-Glucose,             | 14.78 | 0.03 | -1.08 | 1.09 | C22H55NO6Si5     |
| valeric acid           | 11.44 | 0.01 | -1.03 | 1.09 | C9H19O3Si        |
| Propargyl Alcohol      | 17.78 | 0.01 | 1.02  | 1.27 | C6H12OSi         |
| D-(+)-Maltose          | 1.21  | 0.01 | 0.27  | 1.10 | C12 H22 O11      |
| L-Aspartic acid        | 1.31  | 0.00 | 1.14  | 1.19 | C4 H7 N O4       |
| L-Iditol               | 1.13  | 0.00 | -1.65 | 1.17 | C6 H14 O6        |
| L-Phenylalanine        | 1.18  | 0.00 | 1.12  | 1.16 | C9 H11 N O2      |
| pyridin-2-amine        | 5.03  | 0.02 | -1.25 | 1.02 | C5H6N2           |
| Oxyisocyclointegrin    | 1.25  | 0.00 | -1.91 | 1.02 | C21H20O7         |
| Phoxim                 | 1.15  | 0.00 | -2.53 | 1.02 | C12H15N2O3PS     |
| Pipecolic acid         | 1.15  | 0.00 | 1.98  | 1.01 | C6 H11 N O2      |
| Salicylamide           | 1.14  | 0.00 | -2.06 | 1.01 | C7 H7 N O2       |
| $\alpha$ -Lactose      | 3.43  | 0.02 | -0.40 | 1.01 | C12 H22 O11      |
| Tetradecanoic acid     | 21.09 | 0.01 | 1.23  | 1.10 | C3(C13)14H36O2Si |
| Acrylamide             | 11.44 | 0.05 | 1.25  | 1.15 | C3H5NO           |
| Decanoic acid          | 9.17  | 0.00 | 1.37  | 1.11 | C18H38O2Si       |
| Glutaric acid          | 11.92 | 0.04 | 1.40  | 1.10 | C11H24O4Si2      |
| Valeric acid           | 21.57 | 0.00 | 1.40  | 1.05 | C9H19O3Si        |
| Phenylalanine          | 16.24 | 0.04 | 1.51  | 1.28 | C9 H11 N O2      |
| Penicillamine          | 8.93  | 0.00 | 1.73  | 1.32 | C5H11NO2S        |
| Alanine                | 10.88 | 0.07 | 1.76  | 1.01 | C21H30F3NO3      |
| 3-indolepyruvic acid   | 24.38 | 0.00 | 1.79  | 1.06 | C11H9NO3         |
| Octadecanamide         | 15.29 | 0.02 | 2.05  | 1.71 | C22H44N2O2       |
| Chloroacetic acid      | 16.60 | 0.00 | 2.10  | 1.06 | C2H3ClO2         |
| Glycine                | 8.39  | 0.00 | 2.19  | 1.29 | C2H5NO2          |
| Pyrimidine             | 21.84 | 0.00 | 2.24  | 1.19 | C4H4N2           |
| Arginine               | 22.46 | 0.00 | 2.43  | 1.04 | C15H35N3O2Si3    |
| Phenylalanine          | 14.67 | 0.03 | 2.56  | 1.02 | C9 H11 N O2      |
| Tromethamine,          | 11.85 | 0.00 | 2.64  | 1.35 | C16H43NO3Si4     |
| Cyclohexane            | 18.05 | 0.00 | 2.69  | 1.01 | C18H36           |
| l-Alanine              | 17.26 | 0.00 | 2.92  | 1.04 | C21H30F3NO3      |
| Homocystine            | 22.52 | 0.04 | 2.95  | 1.11 | C4H9NO2S         |
| l-Proline              | 21.47 | 0.00 | 3.03  | 1.05 | C5H9NO2          |
| Leucine                | 21.72 | 0.00 | 3.26  | 1.12 | C6H13NO2         |
| Butanoic acid,         | 17.39 | 0.00 | 3.30  | 1.08 | C13H32O4Si3      |
| Acetic acid            | 15.58 | 0.01 | 4.18  | 1.19 | C14H24O3Si2      |
| Sarcosine              | 17.25 | 0.00 | 4.31  | 1.06 | C9H23NO2Si2      |
| Aminohippuric acid     | 9.69  | 0.00 | 4.63  | 1.09 | C15H24N2O3Si     |
| purine                 | 18.89 | 0.00 | 5.12  | 1.13 | C10H13N5         |
| Proline                | 19.15 | 0.00 | 6.74  | 1.13 | C5 H9 N O2       |
| Acetoacetic acid       | 17.25 | 0.00 | 8.08  | 1.12 | C4H6O3           |
| Penicillic-Acid        | 9.52  | 0.00 | 2.92  | 1.09 | C8 H10 O4        |
| L-Methionine Sulfoxide | 8.74  | 0.00 | 2.92  | 1.02 | C5H11NO3S        |
| Atenolol               | 4.84  | 0.14 | 1.03  | 1.07 | C14H22N2O3       |

|                      |       |      |       |      |                 |
|----------------------|-------|------|-------|------|-----------------|
| carboxylic acid      | 18.68 | 0.01 | 2.14  | 1.01 | C19H24N2O5      |
| acetic acid          | 5.76  | 0.00 | 2.58  | 1.41 | C14H24O3Si2     |
| 2-Methylnicotinamide | 1.47  | 0.00 | -0.07 | 1.21 | C7H8N2O         |
| D-glucopyranoside    | 1.21  | 0.04 | 1.75  | 1.09 | C15 H20 O8      |
| Fluxapyroxad         | 5.58  | 0.09 | 1.31  | 1.01 | C18H12F5N3O     |
| Adenine              | 1.17  | 0.00 | 1.41  | 1.16 | C5 H5 N5        |
| Adenosine            | 1.17  | 0.00 | -1.95 | 1.19 | C11 H15 N5 O3 S |
| Adipic acid          | 2.90  | 0.00 | -6.33 | 1.15 | C6H10O4         |
| Anabasine            | 4.88  | 0.00 | -6.33 | 1.11 | C10H14N2        |

Table 3 Monitored ion pairs, retention times, and collision energies for each compound

| Name | Precursor Ion | Product Ion | Name     | Precursor Ion | Product Ion | t <sub>R</sub> | Collision energy |
|------|---------------|-------------|----------|---------------|-------------|----------------|------------------|
| Gly  | 132.05        | 76.1        | Gly-D5   | 136.9         | 41.1        | 2.99           | 30               |
| Ala  | 146           | 42.85       | Ala-D4   | 150           | 46.85       | 3.3            | 12               |
|      |               | 44.05       |          |               | 48.05       |                | 13               |
| Ser  | 162.05        | 42.05       | Ser-D3   | 165.05        | 45.05       | 3.01           | 24               |
|      |               | 60.05       |          |               | 63.05       |                | 13               |
| Pro  | 172           | 70          | Pro-D3   | 175           | 73          | 3.53           | 10               |
| Val  | 174.05        | 55          | Val-D8   | 182.05        | 63          | 3.81           | 23               |
|      |               | 72.05       |          |               | 80.05       |                | 12               |
| Thr  | 176.05        | 56.05       | Thr-D2   | 178.05        | 58.05       | 3.22           | 16               |
|      |               | 74.05       |          |               | 76.05       |                | 13               |
| Leu  | 188.05        | 30.1        | Leu-13c  | 189.05        | 31.1        | 4.12           | 18               |
|      |               | 86.05       |          |               | 87.05       |                | 12               |
| Ile  | 188.05        | 69.1        | Ile-D10  | 198.05        | 79.1        | 4.08           | 19               |
|      |               | 86.05       |          |               | 96.05       |                | 12               |
| Asn  | 189           | 74.05       | Asn-H3   | 192           | 74.9        | 4.13           | 17               |
|      |               | 87.05       |          |               | 107.1       |                | 11               |
| Asp  | 190           | 74.05       | Asp-D3   | 193           | 77.05       | 3.09           | 16               |
|      |               | 88          |          |               | 91          |                | 12               |
| Gln  | 203.05        | 84          | Gln-13C5 | 208.05        | 89          | 3.07           | 19               |
|      |               | 130         |          |               | 135         |                | 14               |
| Met  | 206           | 56.05       | Met-D3   | 209           | 59.05       | 3.91           | 18               |
|      |               | 61          |          |               | 64          |                | 15               |
| His  | 212.05        | 83.05       | His-C6   | 213.9         | 72.7        | 1.36           | 26               |
|      |               | 110.1       |          |               | 116.6       |                | 15               |
| Phe  | 222           | 103.05      | Phe-D8   | 230           | 111.05      | 4.25           | 27               |
|      |               | 120.1       |          |               | 128.1       |                | 16               |
| Arg  | 231.05        | 60.05       | Arg-N4   | 235           | 70.7        | 2.86           | 15               |
|      |               | 70.1        |          |               | 101.2       |                | 24               |
| Tyr  | 238.05        | 91.05       | Tyr-13C6 | 244.05        | 97.05       | 3.84           | 29               |
|      |               | 136.05      |          |               | 142.05      |                | 14               |
| Trp  | 261.05        | 146.05      | Trp-D5   | 266.05        | 151.05      | 4.39           | 18               |
|      |               | 188.1       |          |               | 193.1       |                | 11               |

|     |        |                 |         |       |               |      |          |
|-----|--------|-----------------|---------|-------|---------------|------|----------|
| Cys | 296.95 | 74<br>151.95    | Cys-D6  | 303.5 | 75.5<br>155.5 | 2.87 | 18<br>25 |
| Lys | 203.05 | 84.05<br>130.05 | Lys-D4  | 207   | 56.3<br>86.7  | 3.07 | 18<br>15 |
| Glu | 204    | 84.05<br>130    | Glu-15N | 205   | 85.05<br>131  | 3.36 | 17<br>14 |

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