Table S1. Potential candidates for the discrimination between *X. canadense* *M* and *X. sibiricum* *PW* obtained by VOCs profiles.

| No. | RT (min) | Compounds | Quantifying ion(m/z) | VIP value | Area RSD (%) | Area RSD (%) |
|-----|----------|-----------|---------------------|-----------|--------------|--------------|
|     |          |           |                     |           | *X. canadense* | *X. sibiricum* |
|     |          |           |                     |           | *M*           | *PW*           |
| Acid| 1        | Hexanoic acid| 60                  | 14.2      | 13.7         | 8.51         |
| Alcohol| 2        | 7-Octen-4-ol | 57                  | 3.9       | 16.6         | 12.3         |
| | 3        | 2,3-Butanediol | 45                  | 1.7       | 6.9          | 14.1         |
| | 4        | 2-Octen-1-ol, (E)- | 57                  | 1.7       | 18.0         | 16.6         |
| Aldehyde| 5        | 2,4-Heptadienal, (E,E)- | 81                  | 1.4       | 7.3          | 11.6         |
| | 6        | Benzyl alcohol | 79                  | 1.3       | 13.2         | 8.9          |
| | 7        | Benzeneethanol* | 91                  | 2.9       | 14.7         | 10.5         |
| | 8        | Benzaldehyde* | 106                 | 1.4       | 13.8         | 6.8          |
| | 9        | Benzeneacetaldehyde | 91                  | 2.2       | 13.7         | 8.5          |
| | 10       | 1H-Pyrole-2-carboxaldehyde* | 66                  | 1.2       | 12.9         | 8.8          |
| Cycloalkane| 11       | Decalin, anti-1-methyl-, cis- | 82                  | 3.1       | 18.2         | 6.6          |
| Alkene| 12       | (3E)-3-ETHYL-2-METHYL-1,3-HEXADIENE | 67                  | 1.6       | 12.4         | 9.6          |
| | 13       | 2-Methyl-2-heptene | 69                  | 1.0       | 15.6         | 8.3          |
| Ester| 14       | Hexadecanoic acid, methyl ester | 74                  | 1.1       | 20.5         | 10.2         |
| Ketone| 15       | 1-Penten-3-one, 2-methyl- | 69                  | 1.1       | 21.7         | 7.7          |
| | 16       | 3-Octen-2-one* | 55                  | 2.3       | 13.9         | 9.8          |
| Lactone| 17       | γ-Valerolactone | 56                  | 1.2       | 11.4         | 10.0         |
| | 18       | Butyrolactone* | 86                  | 1.2       | 11.0         | 7.8          |
| | 19       | γ-Caprolactone* | 85                  | 3.6       | 12.3         | 9.7          |
| | 20       | δ-Hexalactone* | 70                  | 1.8       | 12.5         | 9.8          |
| | 21       | Pantolactone* | 71                  | 2.3       | 9.3          | 9.3          |
| | 22       | γ-Octalactone | 85                  | 5.2       | 16.8         | 7.8          |
| | 23       | Carvotanacetone* | 59                  | 2.4       | 9.7          | 10.4         |
| | 24       | 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-2-BENZOFURANYL(3H)-ONE | 111 | 1.5 | 11.4 | 9.8 |
| | 25       | 21.30 | 2-BENZOFURANYL(3H)-ONE | 105 | 1.2 | 10.9 | 11.9 |
| Imide| 26       | 2-Ethyl-3-methylmaleimide | 139 | 1.2 | 9.7 | 9.4 |
| | 27       | Succinimide | 99 | 1.5 | 11.1 | 10.3 |
Table S2. Potential candidates for the discrimination of polar metabolites between *X. canadense* M and *X. sibiricum* PW obtained by GC-TOF MS

| No. | RT (min) | Compound name                      | Quantifying ion(m/z) | VIP value | X. canadense M Area RSD (%) | X. sibiricum PW Area RSD (%) |
|-----|----------|------------------------------------|----------------------|-----------|-----------------------------|-------------------------------|
|     |          | Alcohol                            |                      |           |                             |                               |
| 1   | 7.1      | Ethylene glycol*                   | 147                  | 1.6       | 10.4                        | 9.8                           |
| 2   | 14.7     | Mesoerythritol                     | 217                  | 1.2       | 2.9                         | 5.1                           |
| 3   | 17.2     | L-(-)-Arabitol*                    | 73                   | 10.3      | 14.9                        | 6.0                           |
| 4   | 19.4     | D-Mannitol*                        | 319                  | 3.7       | 12.6                        | 6.2                           |
| 5   | 20.3     | Scylo-inositol*                    | 318                  | 4.4       | 4.3                         | 14.3                          |
| 6   | 20.4     | L-Fucitol                          | 117                  | 1.0       | 3.8                         | 8.1                           |
|     |          | Acid                               |                      |           |                             |                               |
| 7   | 7.2      | N,N-Dimethylglycine 3-Hydroxypropanoic acid | 58 | 1.7 | 16.4 | 11.8 |
| 8   | 9.7      | Hydroxypropanoic acid              | 147                  | 1.3       | 6.94                        | 7.9                           |
| 9   | 12.2     | Succinic acid*                     | 247                  | 1.6       | 3.64                        | 4.1                           |
| 10  | 12.4     | D-Glyceric acid*                   | 189                  | 1.7       | 4.8                         | 9.1                           |
| 11  | 12.7     | Fumaric acid*                      | 245                  | 1.2       | 5.2                         | 5.6                           |
| 12  | 14.5     | Malic acid*                        | 73                   | 10.1      | 7.6                         | 11.2                          |
| 13  | 15.3     | Erythronic acid                    | 73                   | 3.5       | 5.9                         | 13.5                          |
| 14  | 18.1     | Azelaic acid*                      | 55                   | 1.1       | 5.8                         | 7.7                           |
| 15  | 20.1     | Gluconic acid*                     | 333                  | 1.3       | 6.7                         | 19.1                          |
|     |          | Ester                              |                      |           |                             |                               |
| 16  | 10.1     | L-Proline, 1-methyl-, methyl ester | 84                   | 1.6       | 23.1                        | 8.1                           |
|     |          | Ketone                             |                      |           |                             |                               |
| 17  | 18.2     | 2,4-Imidazolidinedione             | 93                   | 1.0       | 12.3                        | 15.9                          |
|     |          | Monosaccharide                     |                      |           |                             |                               |
| 18  | 19.3     | d-Mannose                          | 319                  | 2.4       | 4.1                         | 6.3                           |
| 19  | 32.3     | D-Psicofuranose*                   | 230                  | 1.2       | 13.4                        | 15.5                          |

* Quantitative analysis was performed using their corresponding authentic standards