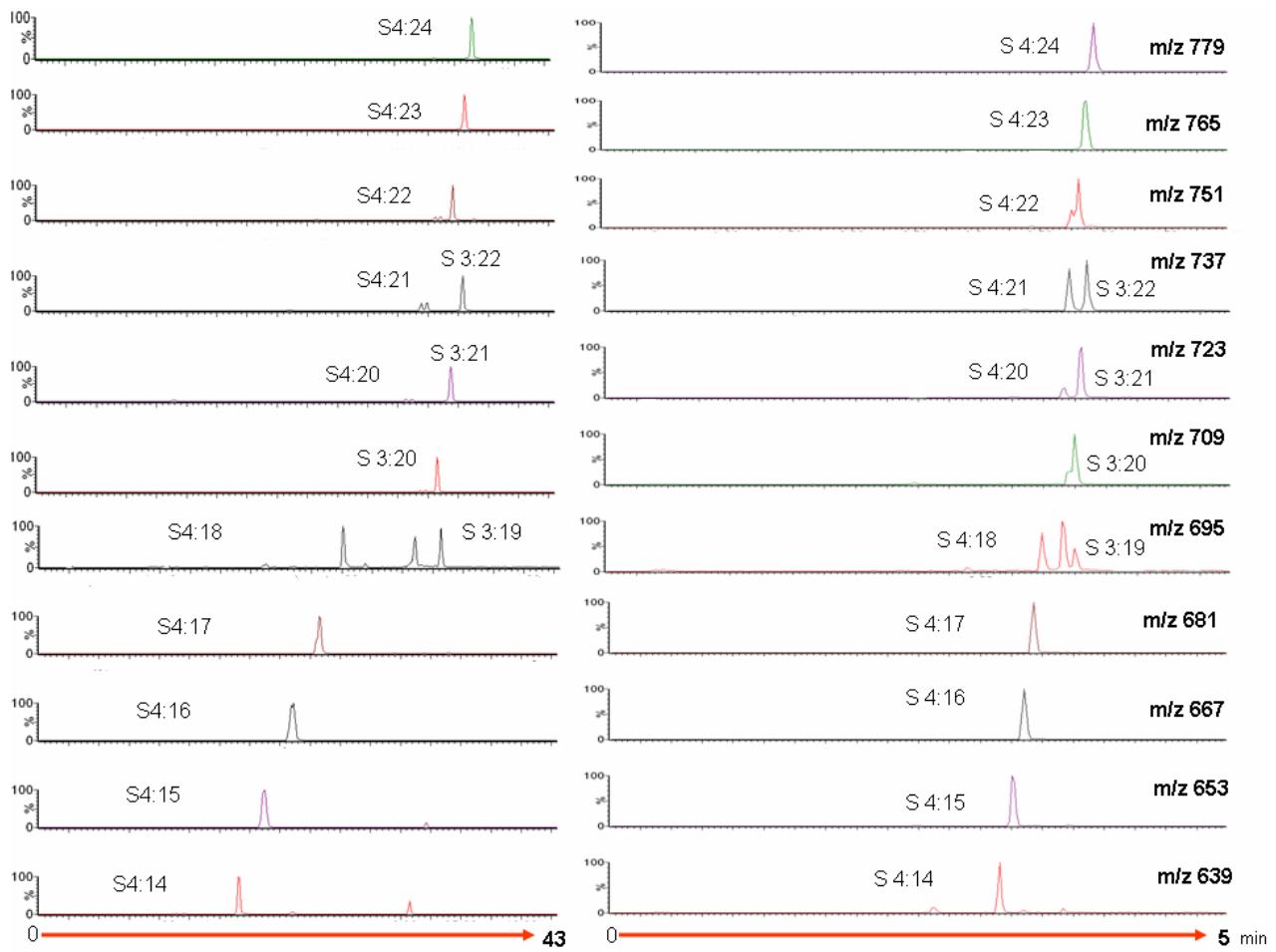
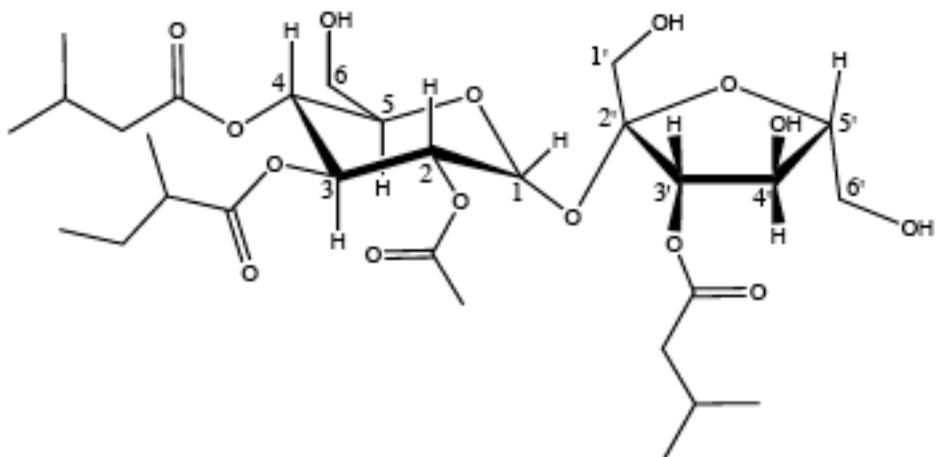


**Figure S1. Schilmiller, Shi et al.**

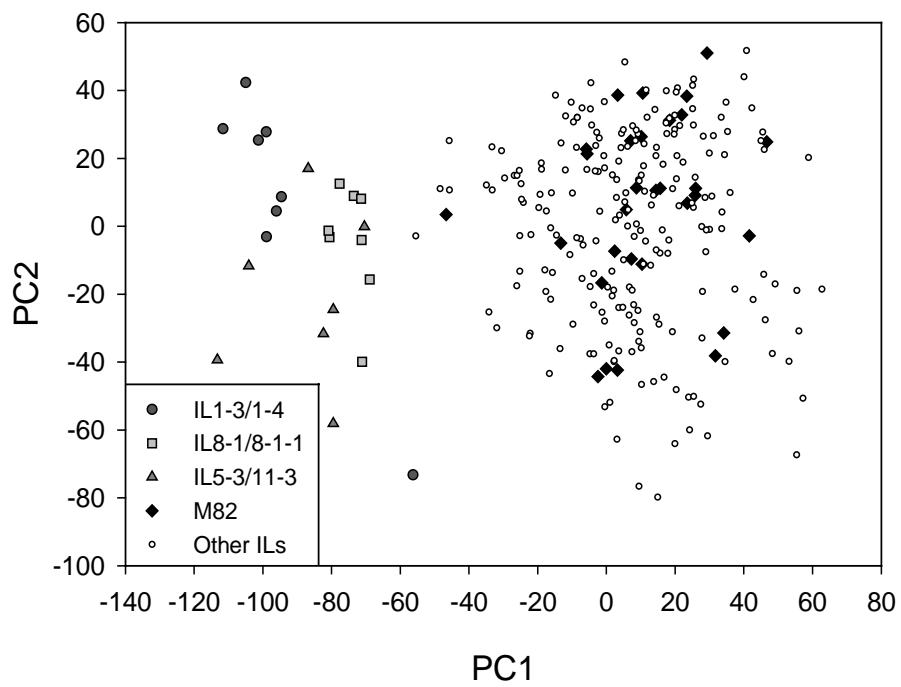


**Figure S2. Schilmiller, Shi et al.**

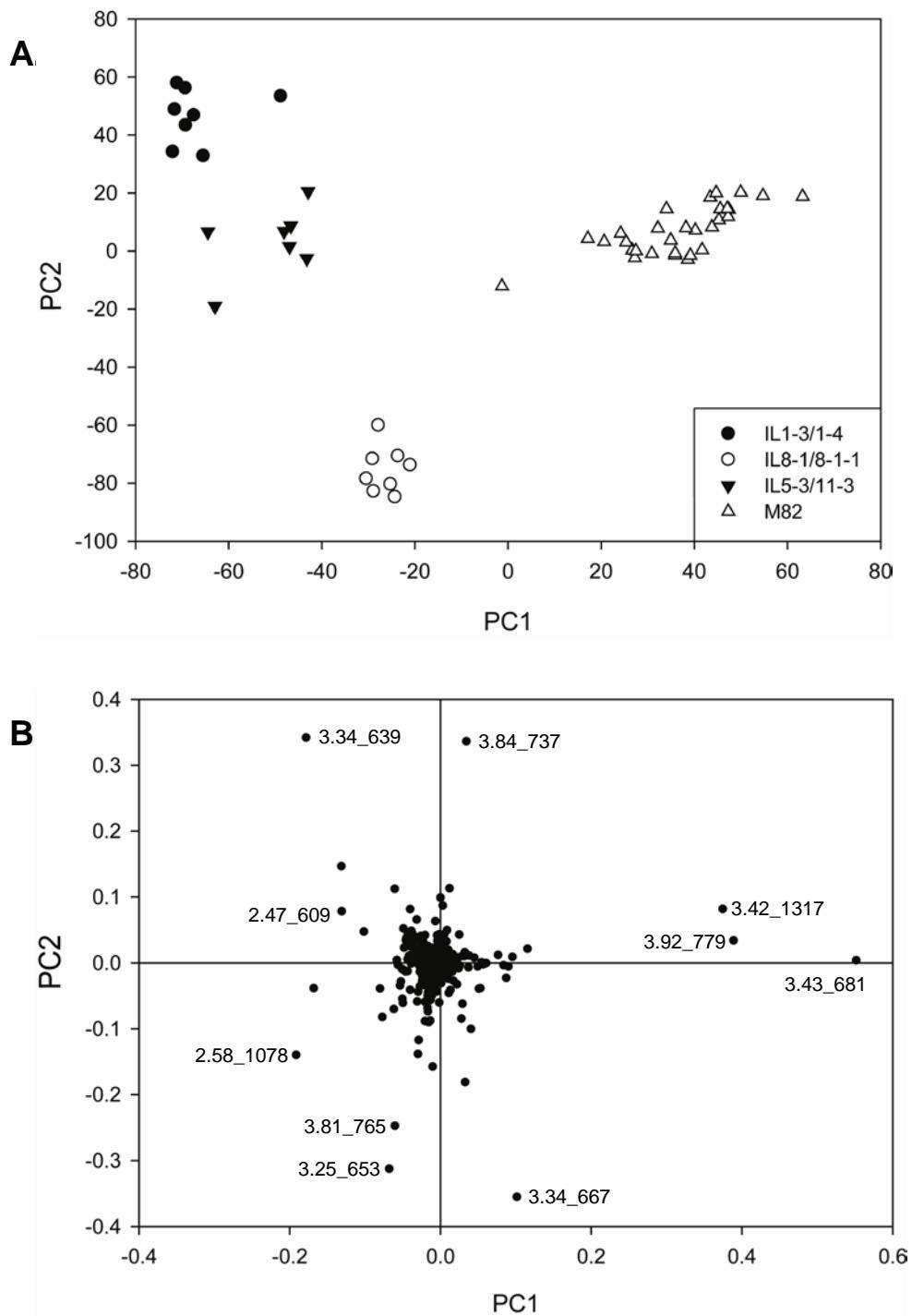


| Carbon # (multiplicity) | <sup>1</sup> H mult. (J, Hz)    | <sup>13</sup> C |
|-------------------------|---------------------------------|-----------------|
| 1 (CH)                  | 5.61 <i>d</i> (3.7)             | 89.3            |
| 2 (CH)                  | 4.85 <i>dd</i> (10.6, 3.7)      | 70.5            |
| 2-O-                    |                                 |                 |
| -1 (CO)                 | ---                             | 170.2           |
| -2 (CH <sub>2</sub> )   | 1.98 <i>s</i>                   | 20.6            |
| 3 (CH)                  | 5.44 <i>dd</i> (10.6, 10.0)     | 68.9            |
| 3-O-                    |                                 |                 |
| -1 (CO)                 | ---                             | 175.4           |
| -2 (CH)                 | 2.29 <i>m</i>                   | 40.9            |
| -2 (-CH <sub>2</sub> )  | 1.03 <i>d</i> (7.0)             | 16.4            |
| -3 (CH <sub>2</sub> )   | 1.56, 1.37 <i>sext</i> (7.0)    | 26.5            |
| -4 (CH <sub>2</sub> )   | 0.81 <i>t</i> (7.4)             | 11.4            |
| 4 (CH)                  | 4.92 <i>dd</i> (10.2, 10.0)     | 68.5            |
| 4-O-                    |                                 |                 |
| -1 (CO)                 | ---                             | 172.2           |
| -2 (CH <sub>2</sub> )   | 2.1 - 2.4 <i>m</i> <sup>b</sup> | 42.9            |
| -3 (CH)                 | 2.15 <i>m</i>                   | 25.8            |
| -4 (CH <sub>2</sub> )   | 0.9 <i>d</i> (7) <sup>a</sup>   | 22.3            |
| -5 (CH <sub>2</sub> )   | 1.0 <i>d</i> (7) <sup>a</sup>   | 22.3            |
| 5 (CH)                  | 4.09 <i>m</i>                   | 71.5            |
| 6 (CH <sub>2</sub> )    | 3.56, 3.60 <i>m</i>             | 61.4            |
| 1' (CH <sub>2</sub> )   | 3.47, 3.58 <i>d</i> (12.3)      | 64.2            |
| 2' (C)                  | ---                             | 103.9           |
| 3' (CH)                 | 5.21 <i>d</i> (7.9)             | 78.7            |
| 3'-O-                   |                                 |                 |
| -1 (CO)                 | ---                             | 174.0           |
| -2 (CH <sub>2</sub> )   | 2.3-2.4 <i>m</i> <sup>b</sup>   | 43.0            |
| -3 (CH)                 | 2.03 <i>m</i>                   | 25.3            |
| -4 (CH <sub>2</sub> )   | 0.91 <i>d</i> (7) <sup>a</sup>  | 22.3            |
| -5 (CH <sub>2</sub> )   | 1.01 <i>d</i> (7) <sup>a</sup>  | 22.3            |
| 4' (CH)                 | 4.45 <i>dd</i> (8.0, 8.0)       | 71.5            |
| 5' (CH)                 | 3.91 <i>m</i>                   | 82.5            |
| 6' (CH <sub>2</sub> )   | 3.70, 3.85 <i>m</i>             | 60.3            |

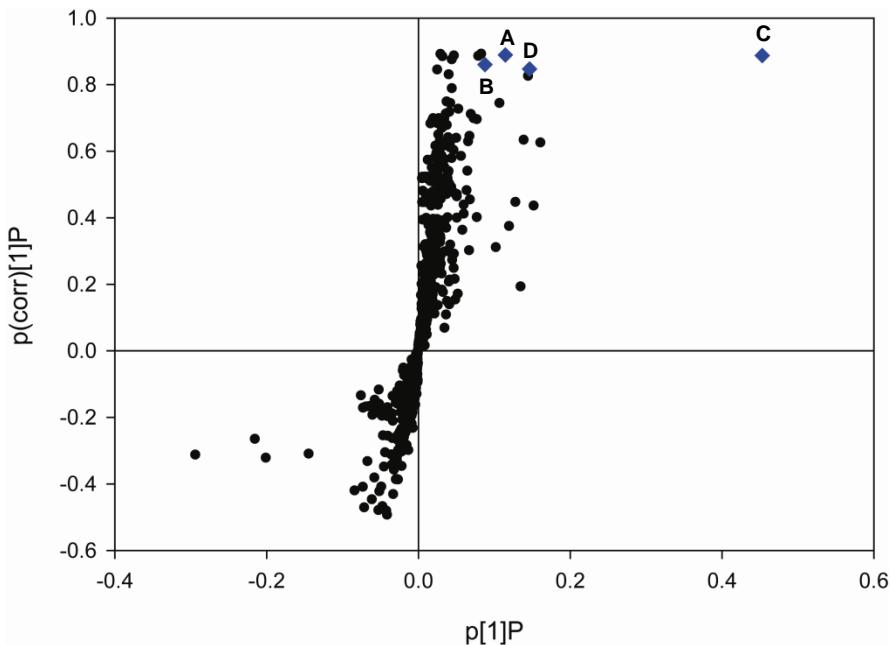
Figure S3. Schilmiller, Shi et al.



**Figure S4 Schilmiller, Shi et al.**

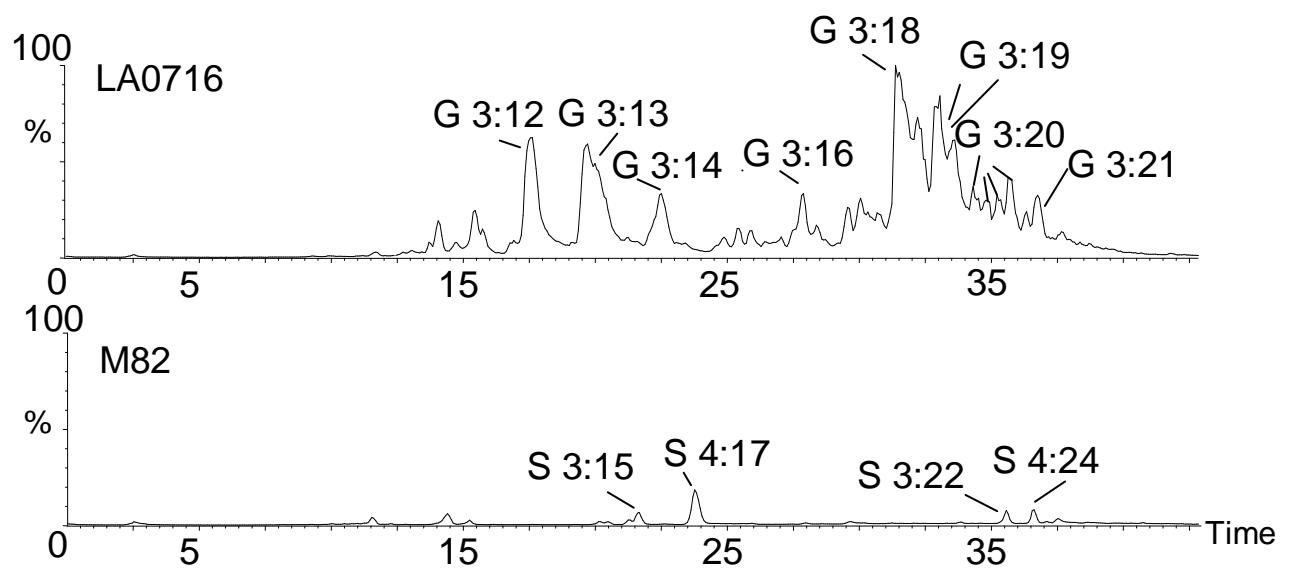


**Figure S5 Schilmiller, Shi et al.**



|   | Retention time_m/z | $p[1]P$ | $p(\text{corr})[1]P$ |
|---|--------------------|---------|----------------------|
| A | 2.51_1066          | 0.114   | 0.889                |
| B | 2.47_1074          | 0.088   | 0.860                |
| C | 2.49_1076          | 0.453   | 0.887                |
| D | 2.60_1094          | 0.146   | 0.847                |

**Figure S6. Schilmiller, Shi et al.**



**Figure S7. Schilmiller, Shi et al.**