

## **Supplementary materials**

### **Chemical Relationship among Genetically Authenticated Medicinal Species of Genus Angelica**

Jung-Hoon Kim<sup>1,‡</sup>, Eui-Jeong Doh<sup>2,‡</sup>, Han-Young Kim<sup>3</sup>, Guemsan Lee<sup>2,4\*</sup>,

<sup>1</sup>Division of Pharmacology, School of Korean Medicine, Pusan National University, Yangsan, 50612, Republic of Korea

<sup>2</sup>Research Center of Traditional Korean Medicine, Wonkwang University, Iksan, 54538, Republic of Korea

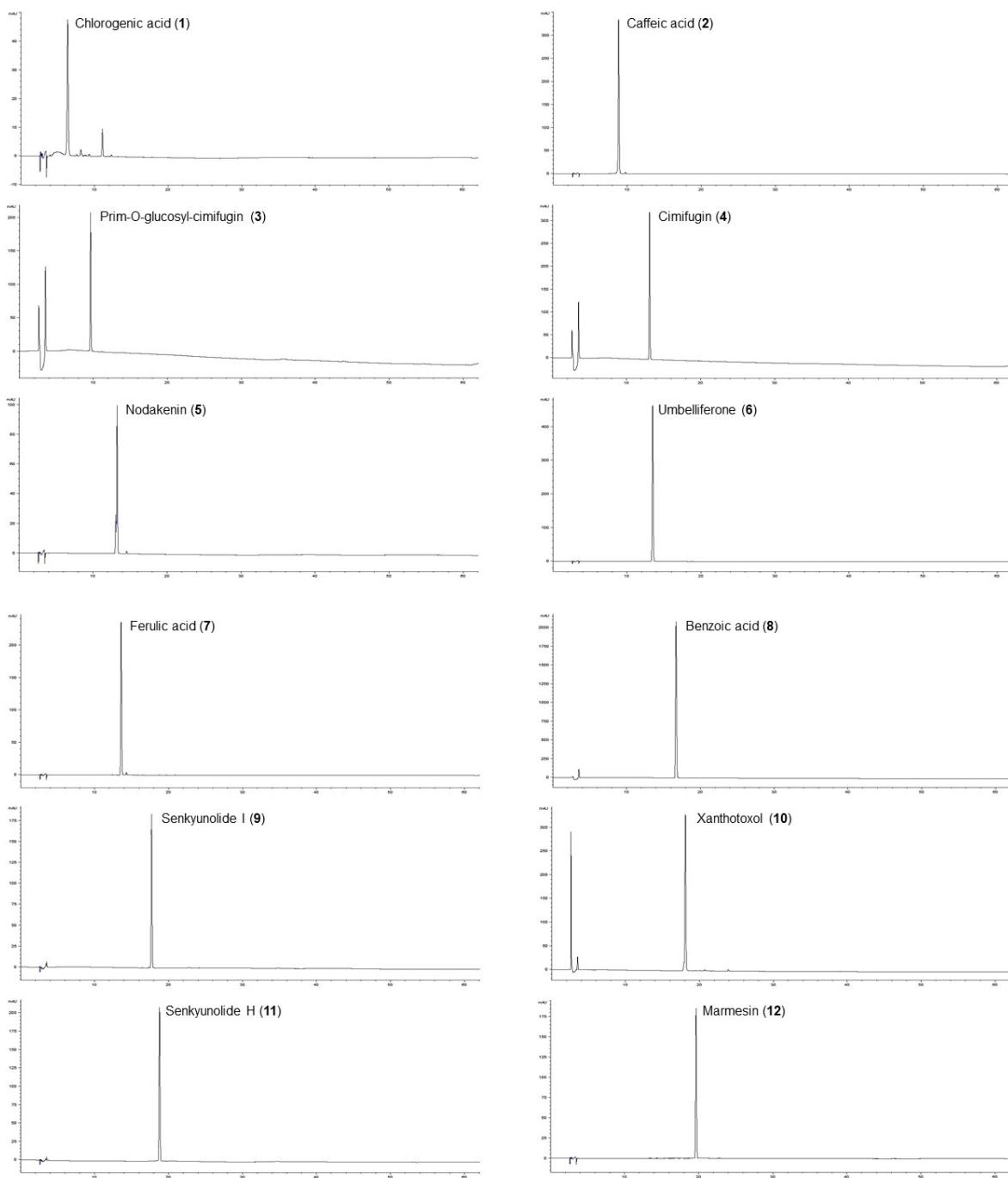
<sup>3</sup>School of Korean Medicine, Pusan National University, Yangsan, 50612, Republic of Korea

<sup>4</sup>Department of Herbology, College of Korean Medicine, Wonkwang University, Iksan, 54538, Republic of Korea

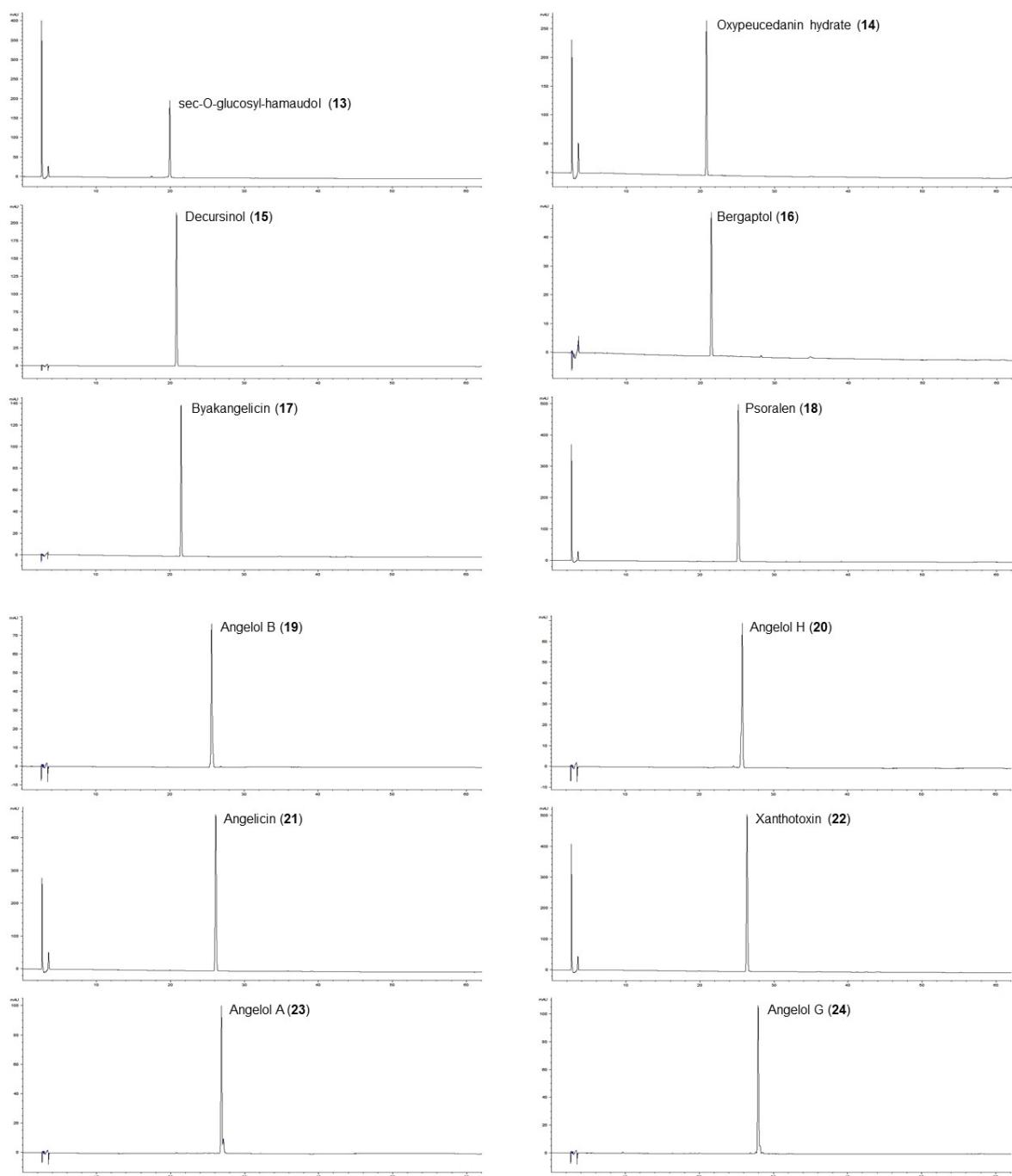
\*Corresponding author at: Department of Herbology, College of Korean Medicine, Wonkwang University, Iksan, 54538, Republic of Korea

E-mail: rasfin@wku.ac.kr

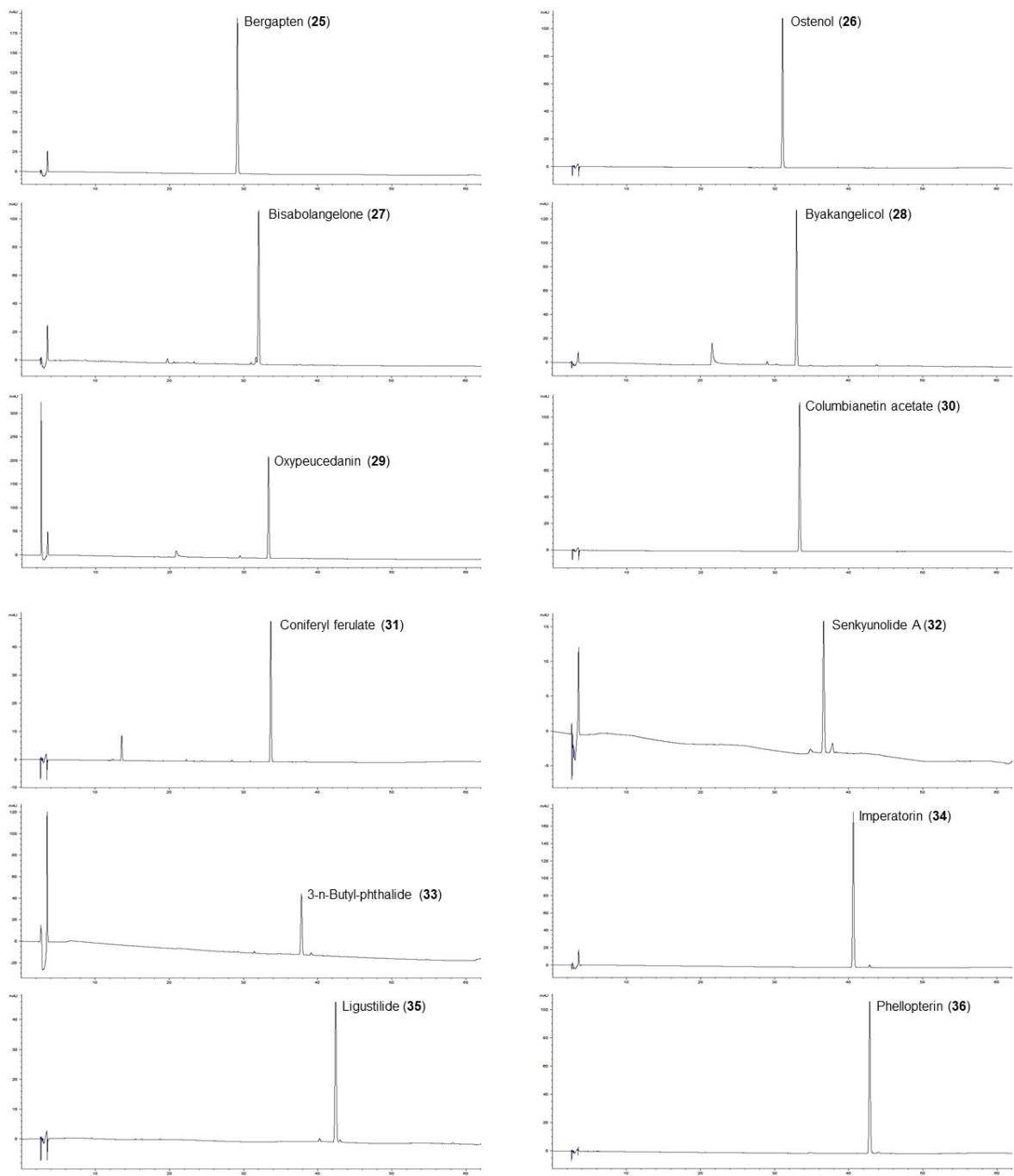
‡These authors contributed equally to this work.



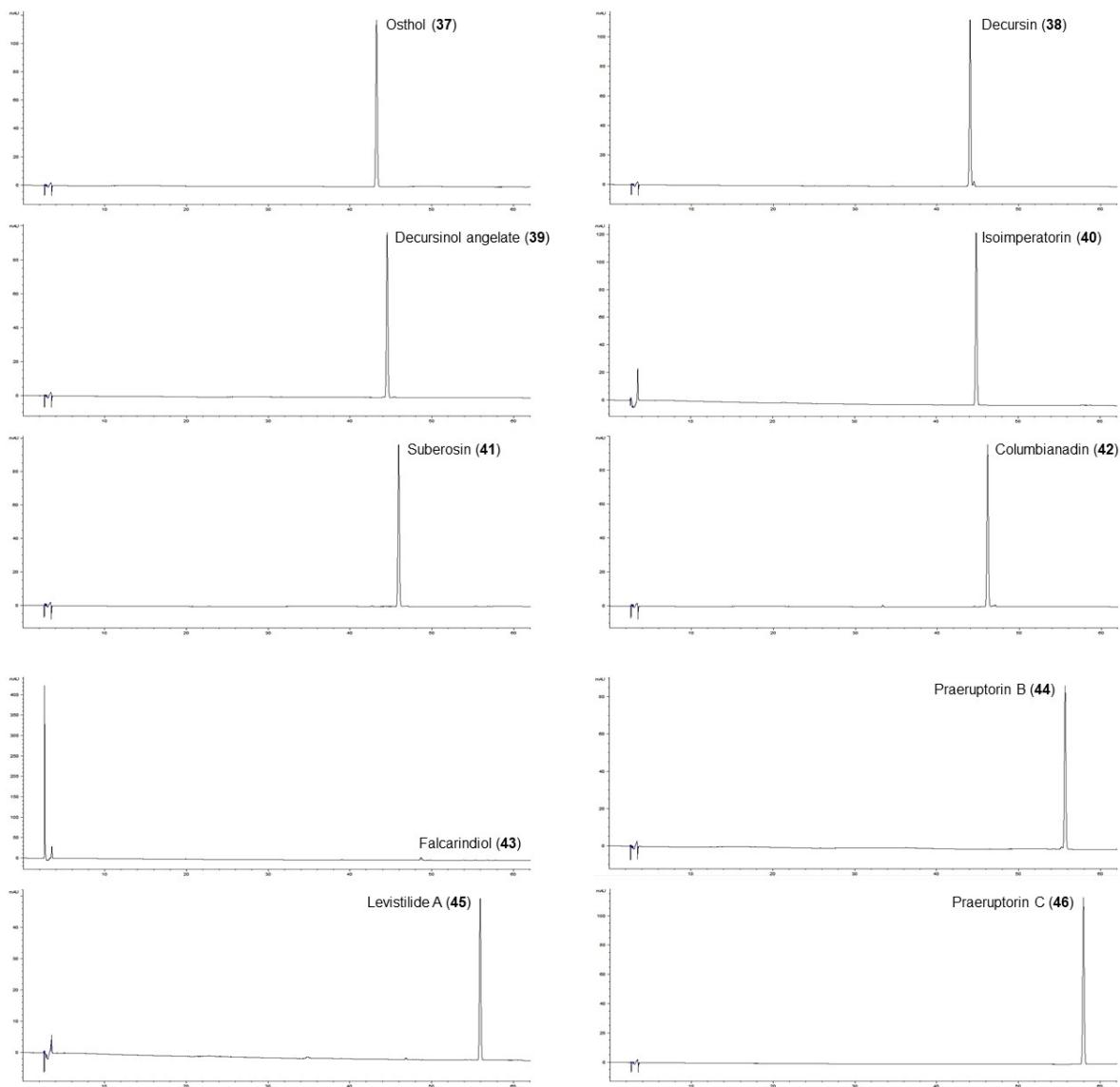
**Figure S1.** Single chromatograms of 46 marker compound.



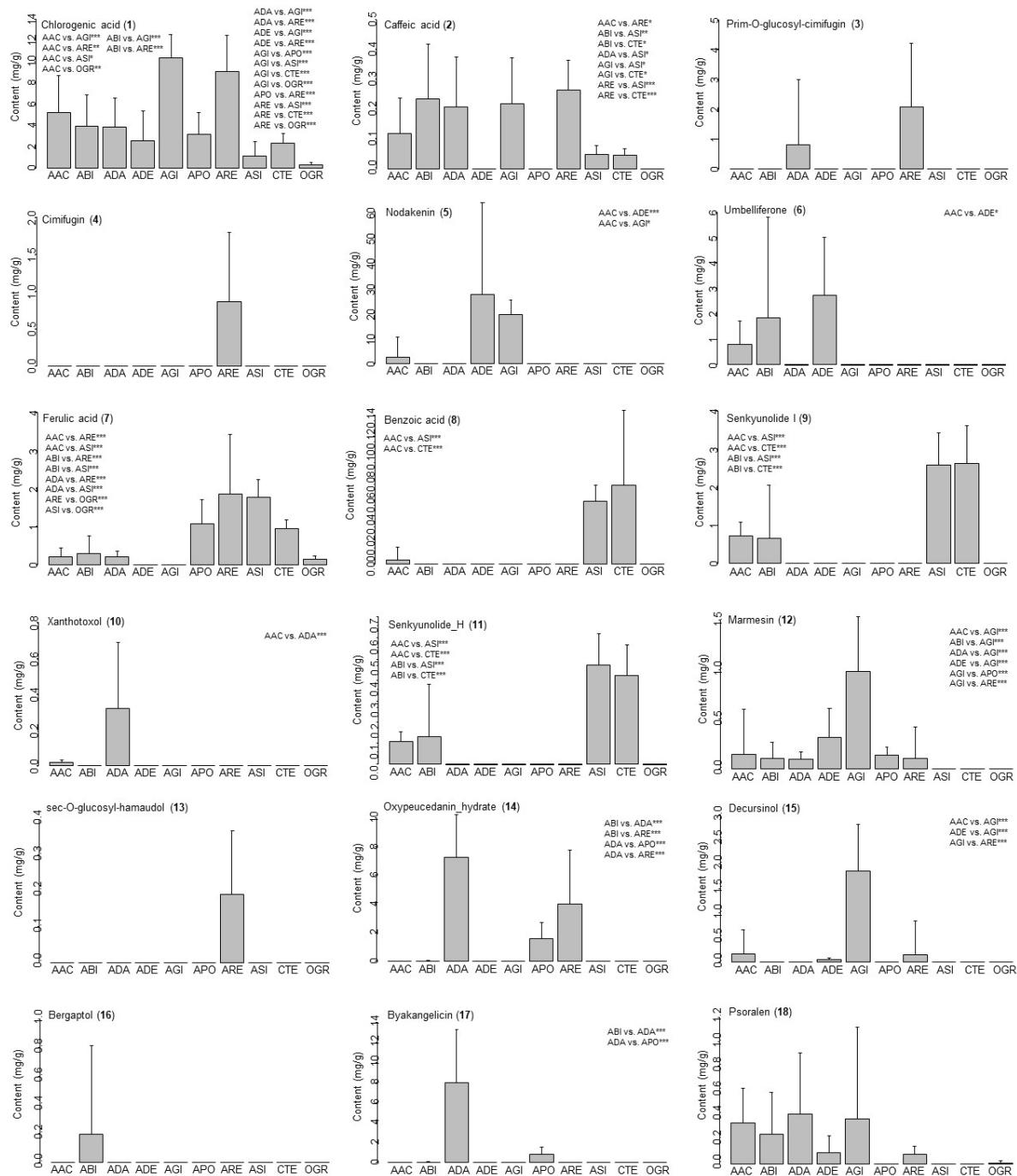
Continued.



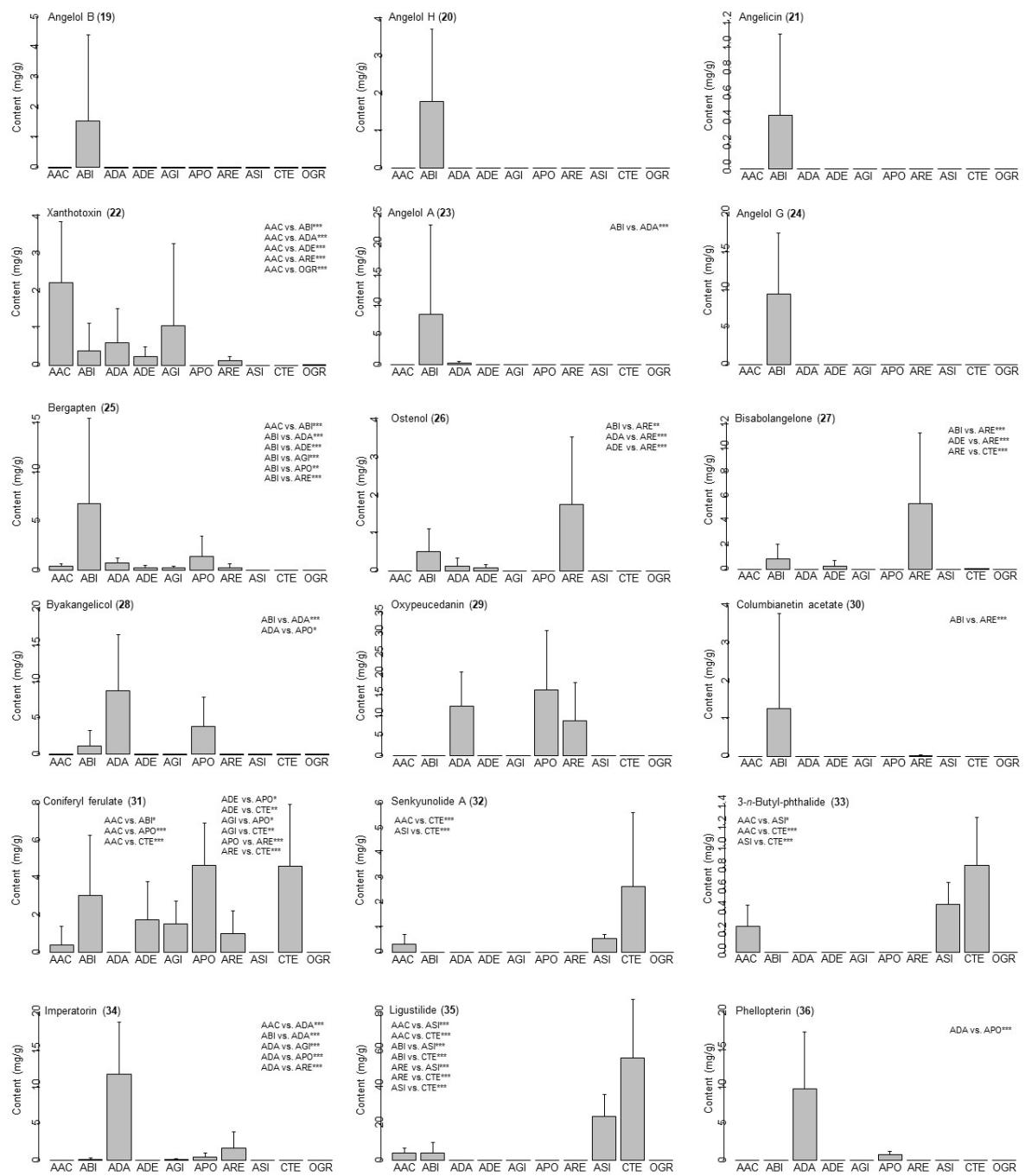
Continued.



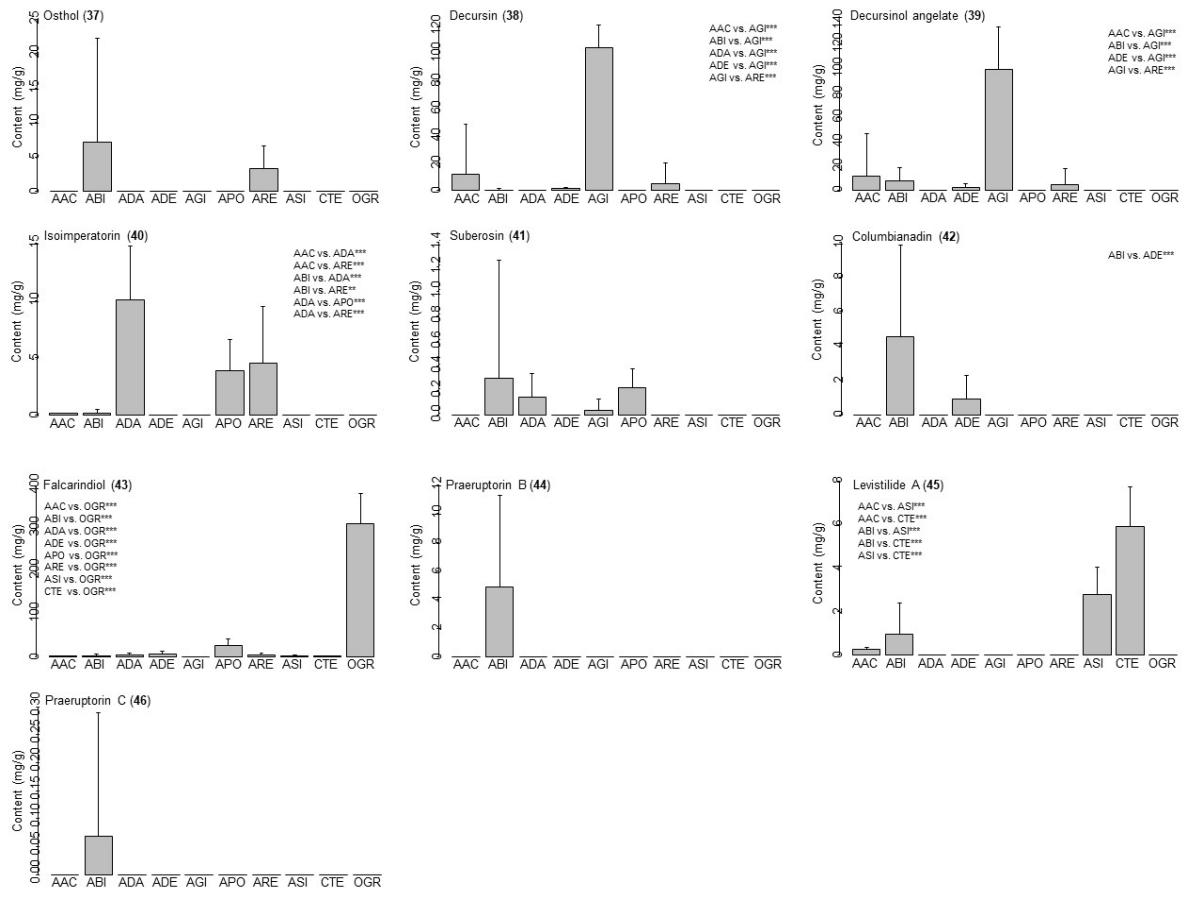
Continued.



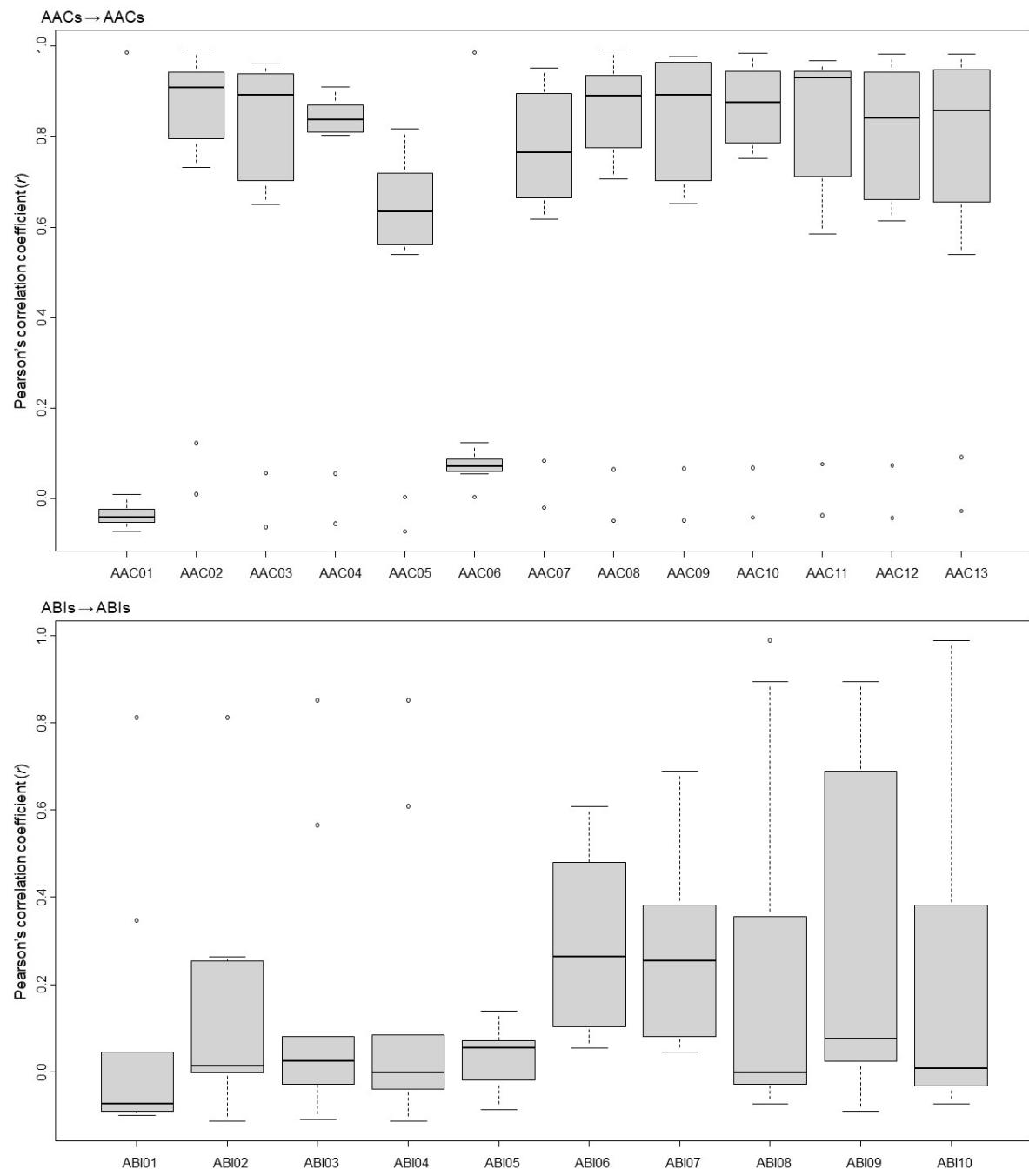
**Figure S2.** Comparison of the contents of the marker compounds among the samples. *Angelica acutiloba* (AAC), *A. biserrata* (ABI), *A. dahurica* (ADA), *A. decursiva* (ADE), *Angelica gigas* (AGI), *A. polymorpha* (APO), *A. reflexa* (ARE), *A. sinensis* (ASI), *Conioselinum tenuissimum* (CTE), and *Ostericum grosseratum* (OGR).



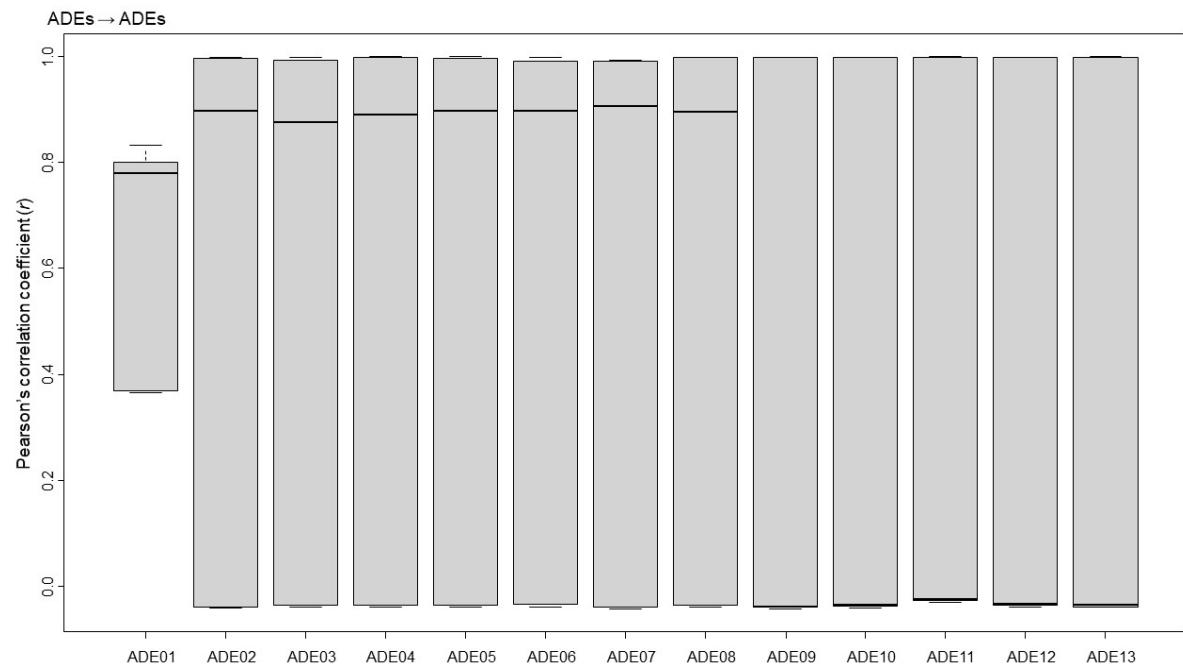
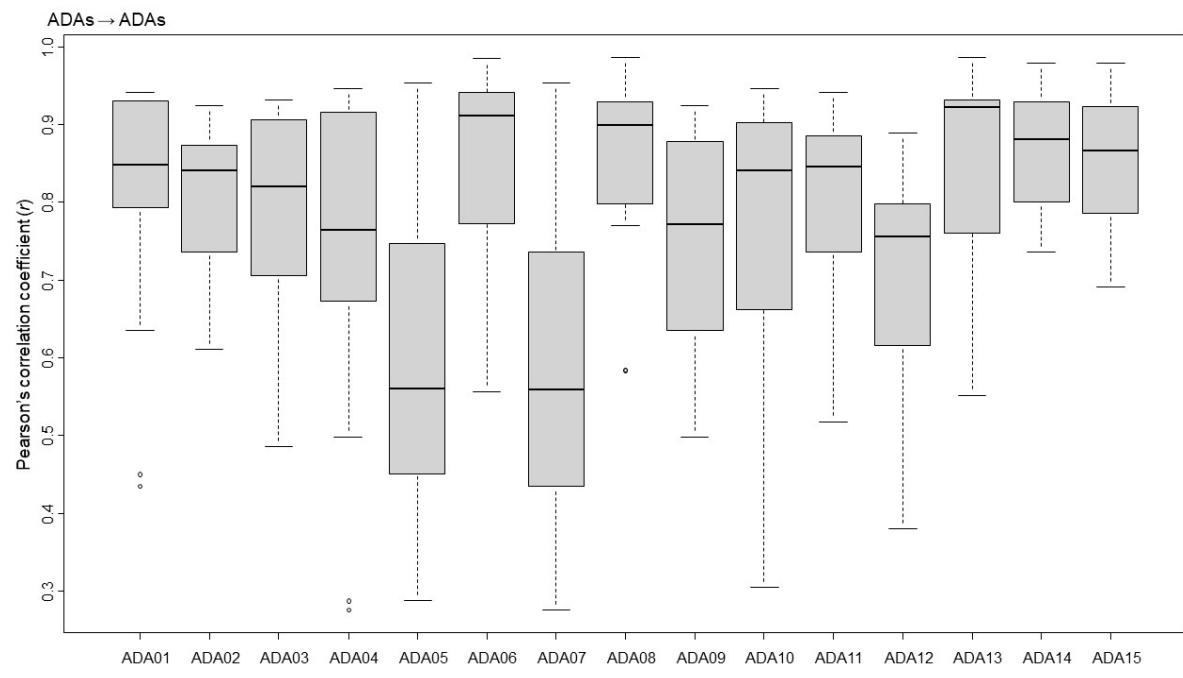
Continued.



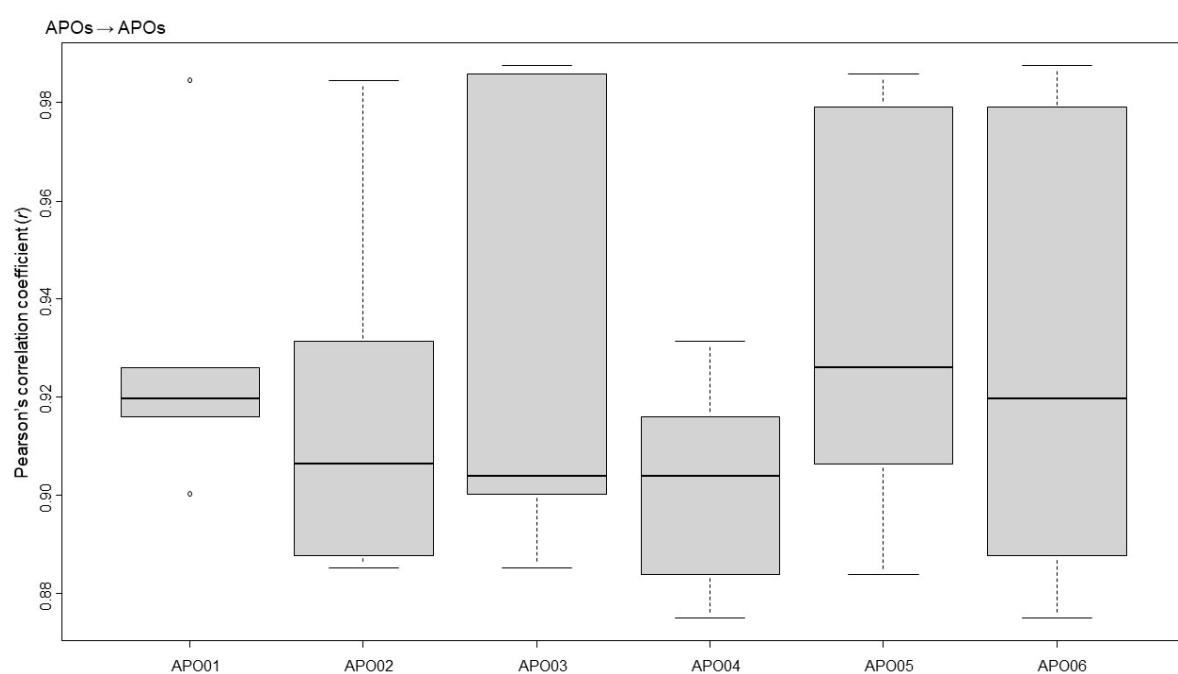
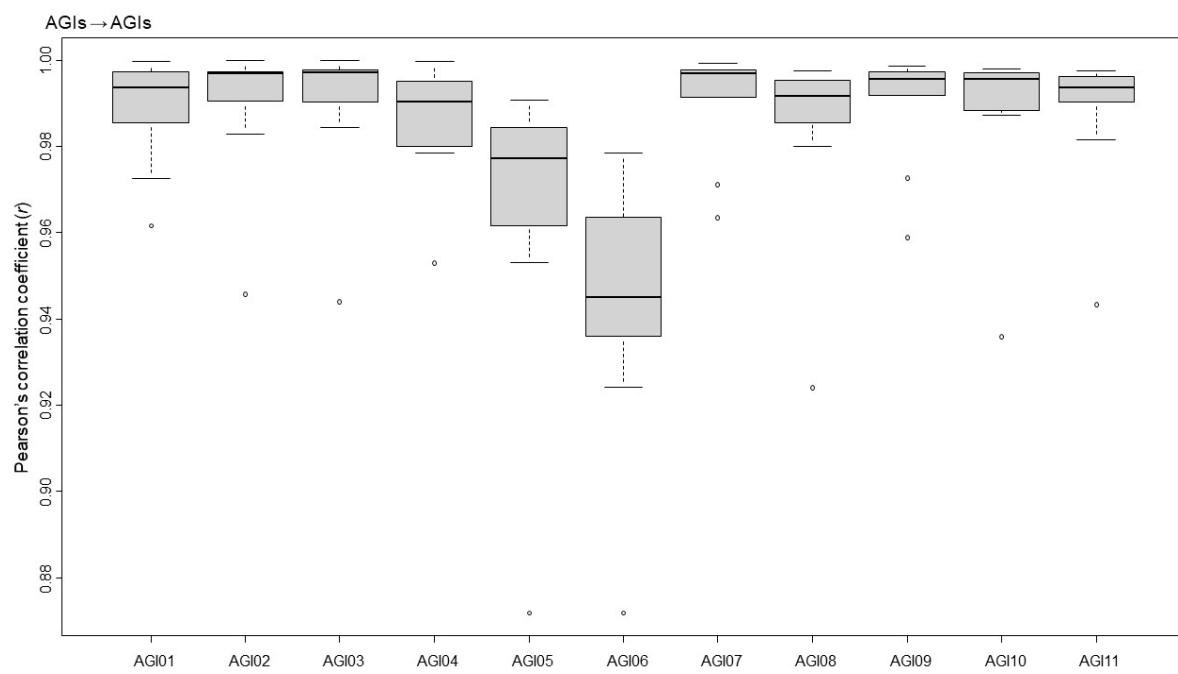
Continued.



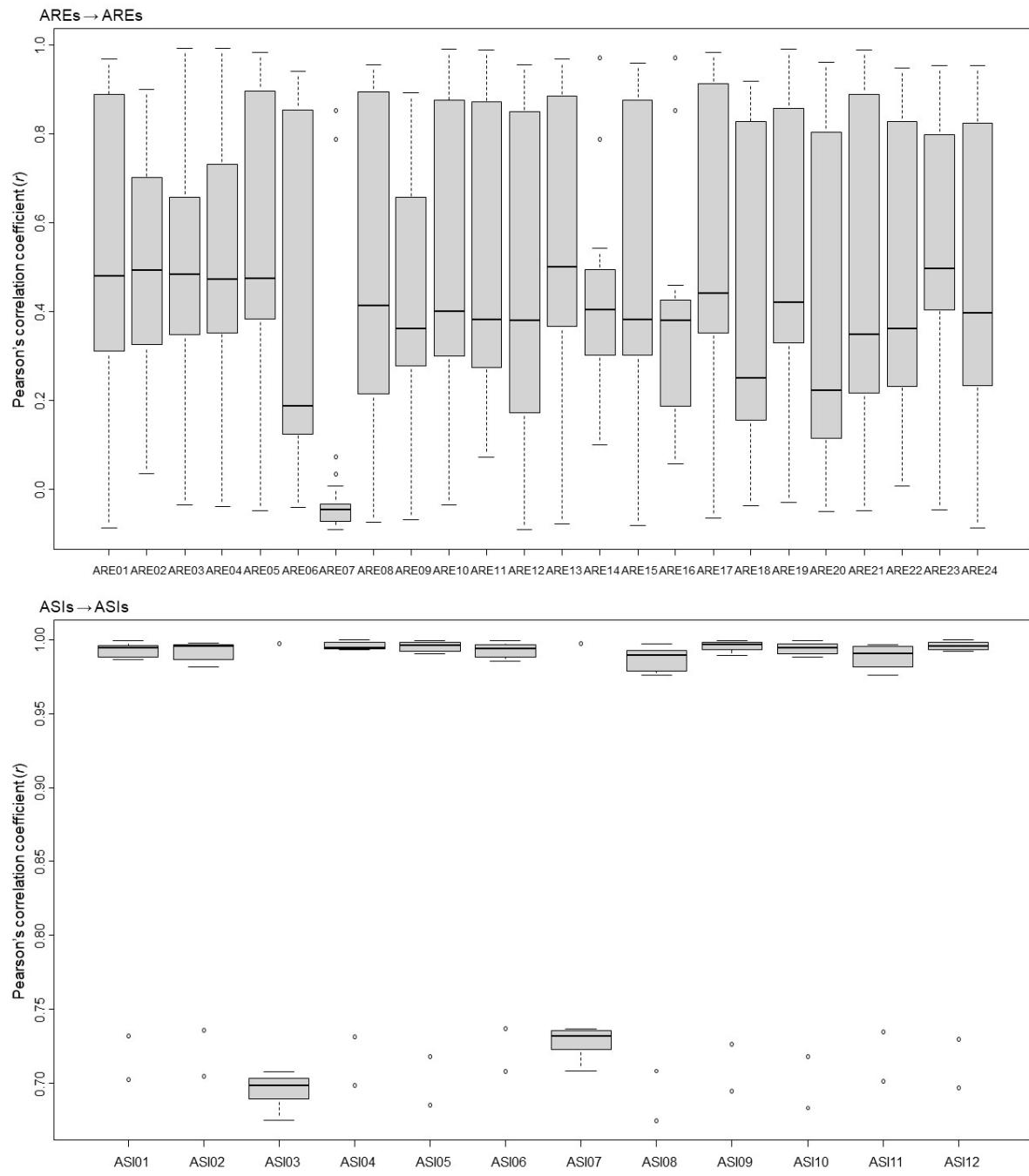
**Figure S3.** Intraspecies Pearson's correlation coefficients among the samples.



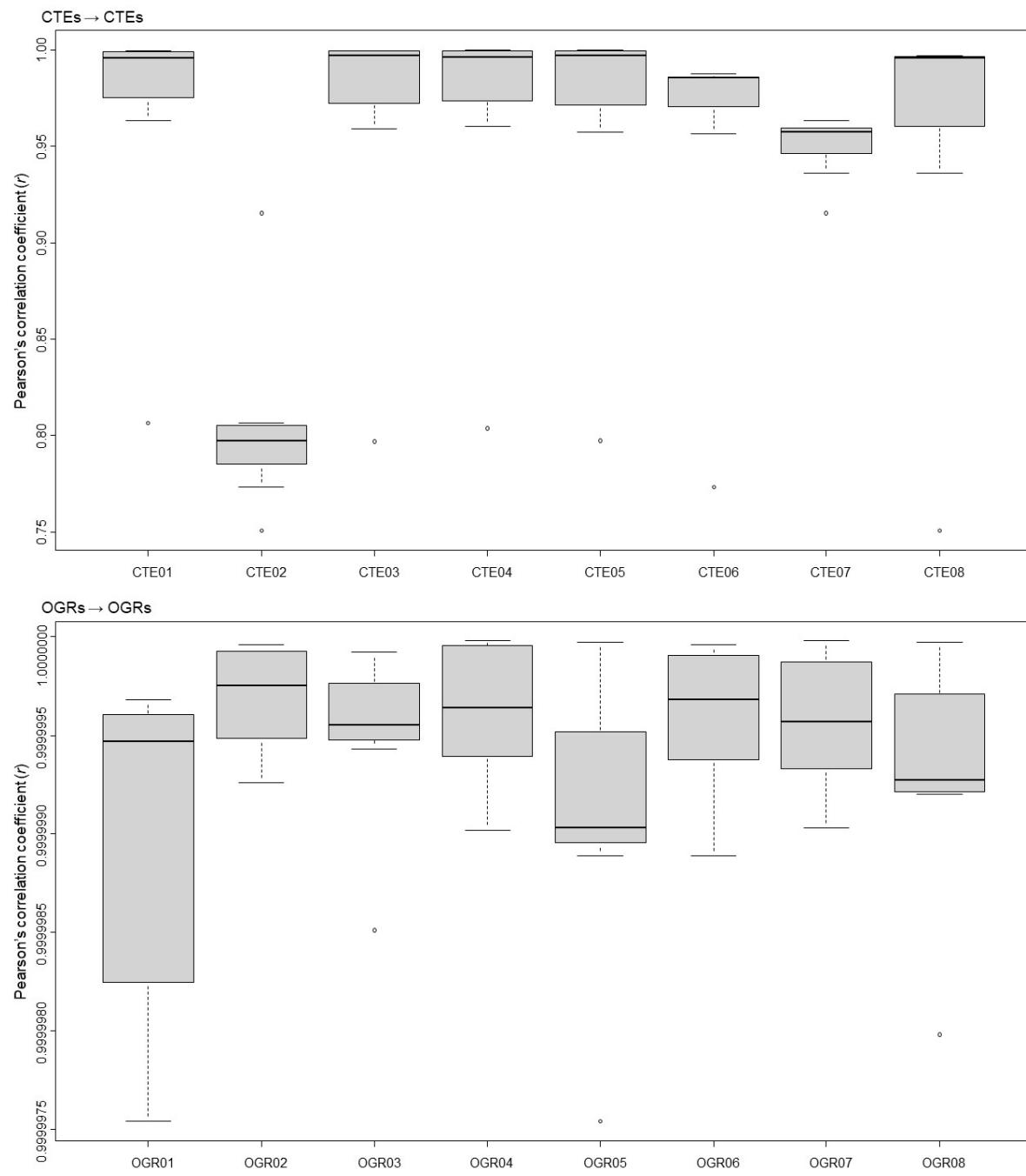
Continued.



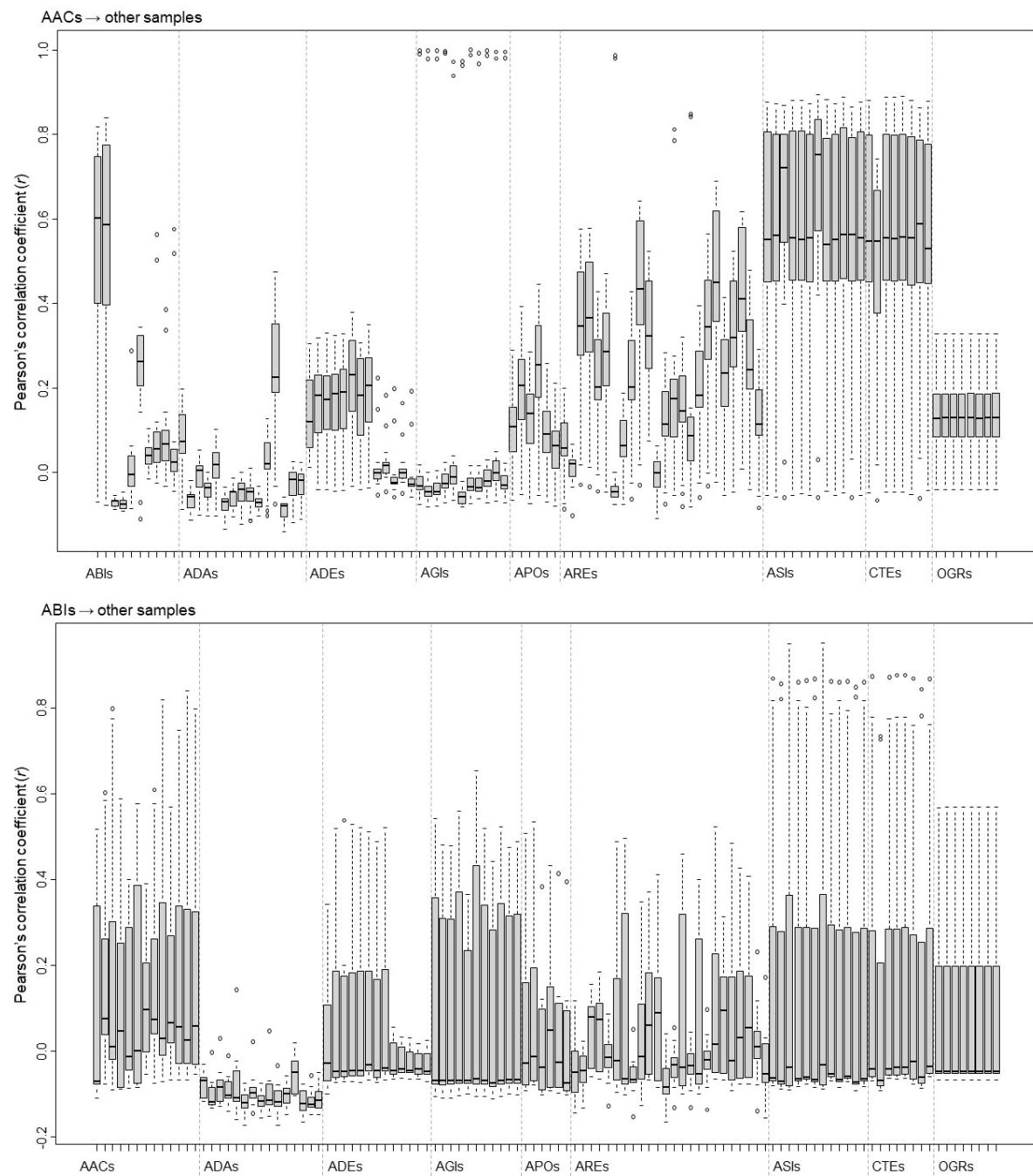
Continued.



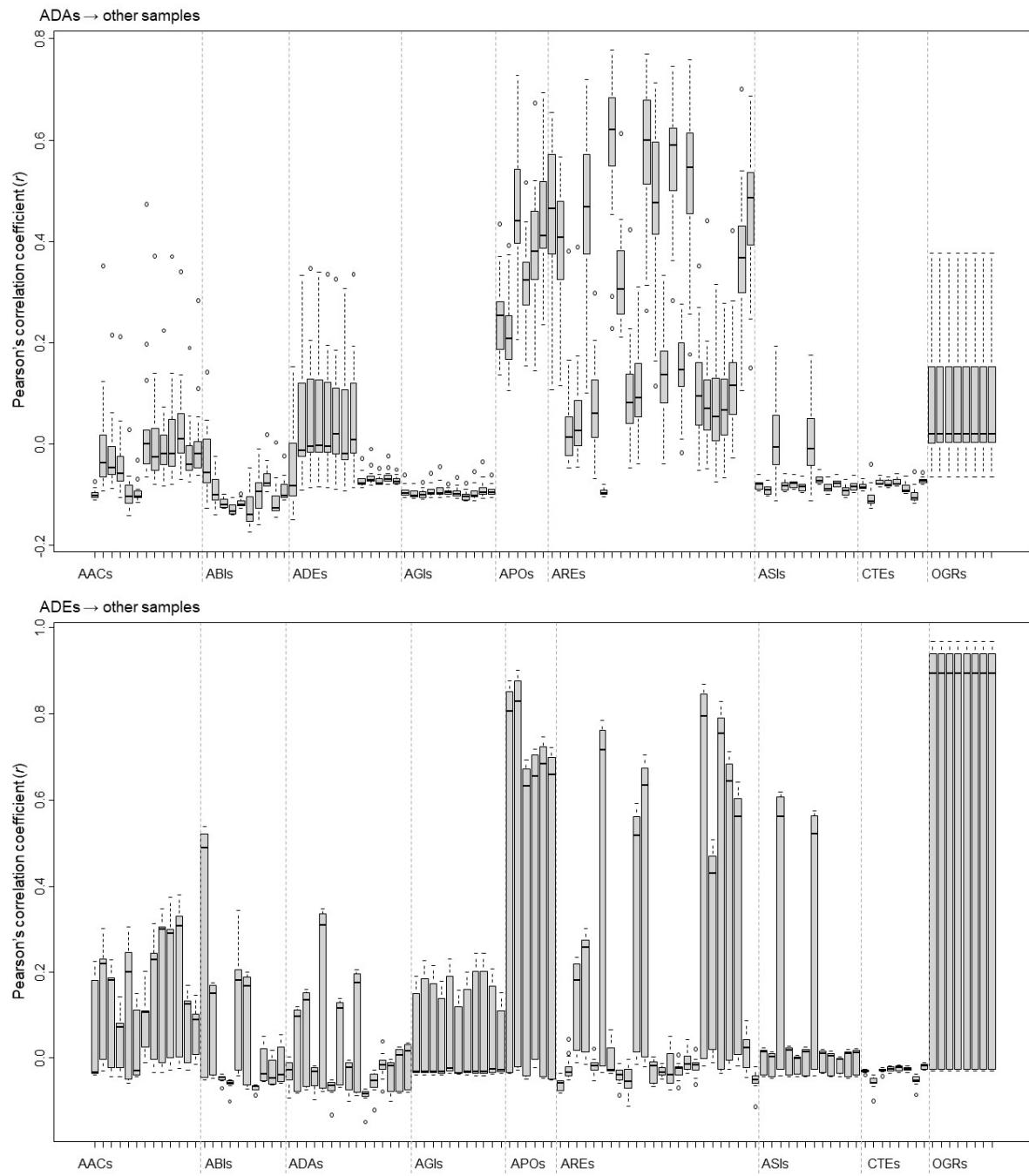
Continued.



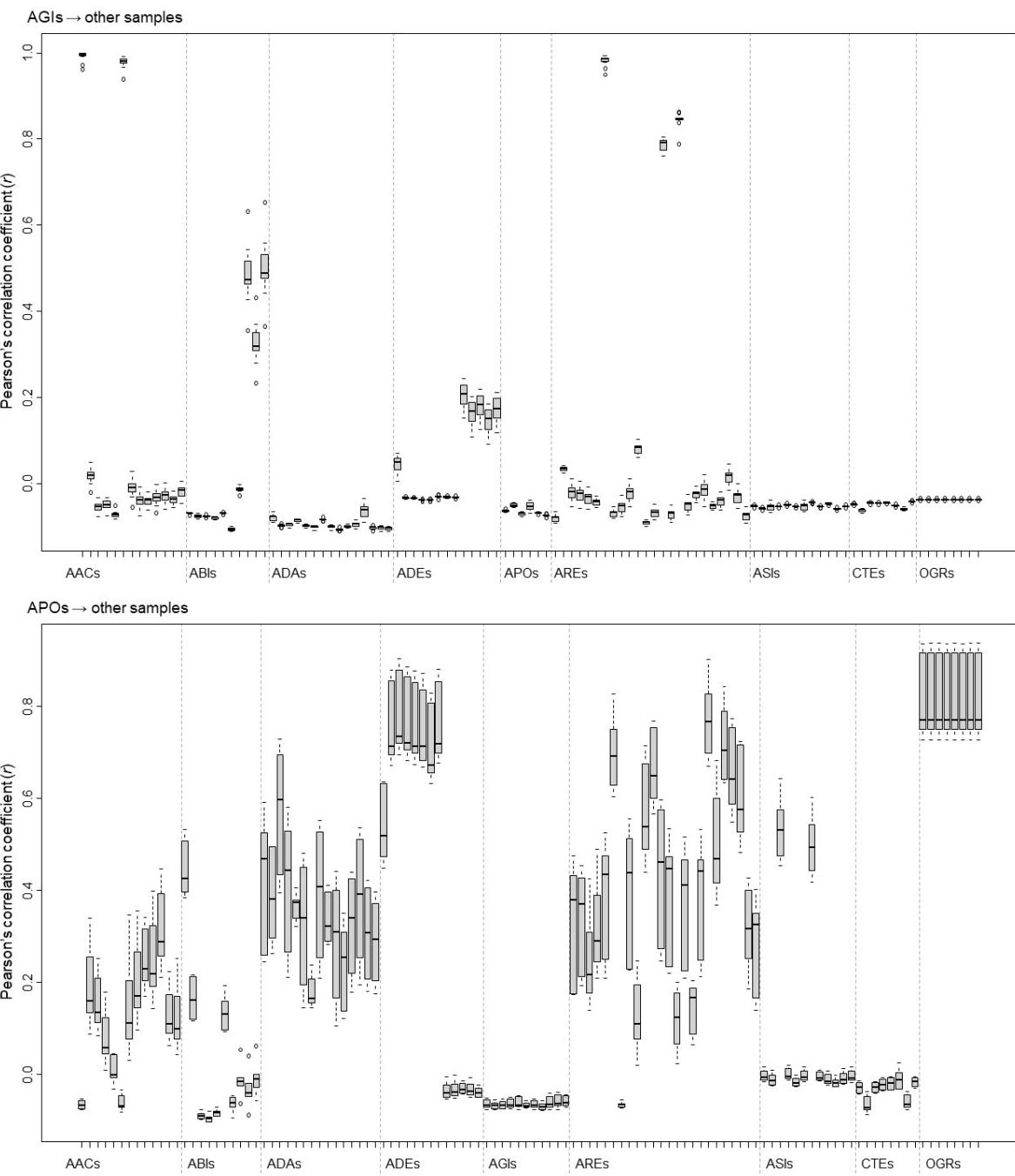
Continued.



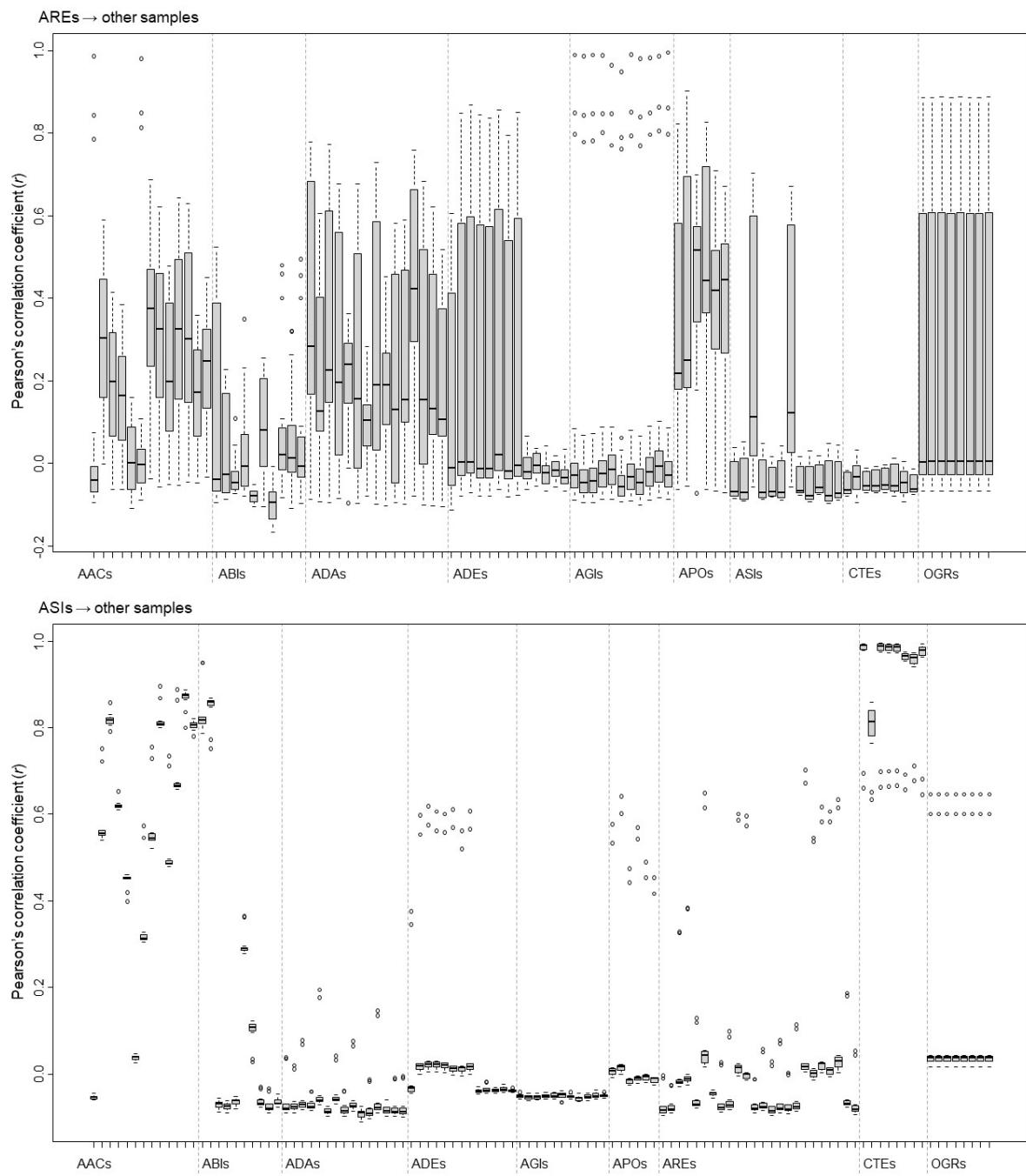
**Figure S4.** Interspecies Pearson's correlation coefficients among the samples.



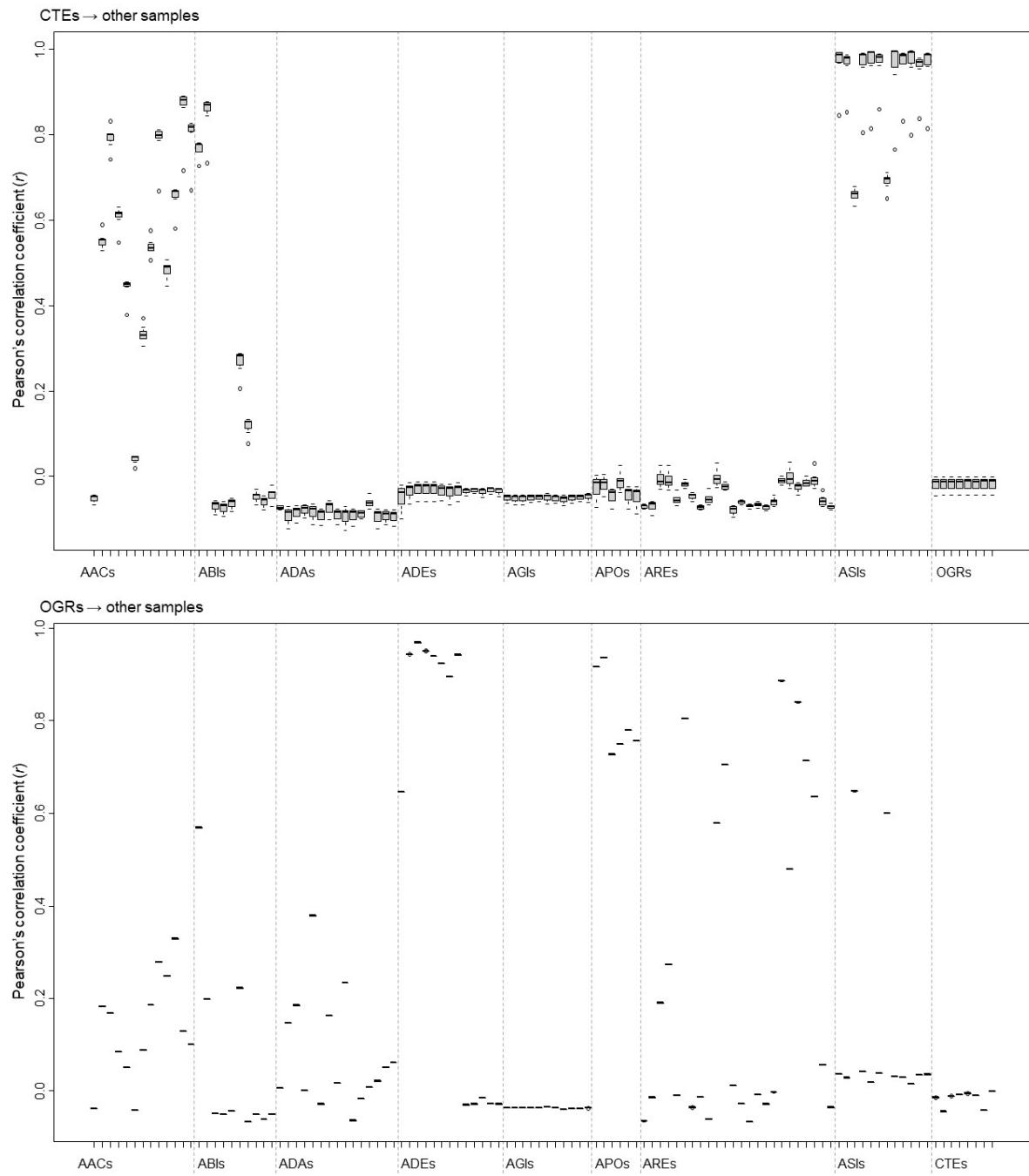
Continued.



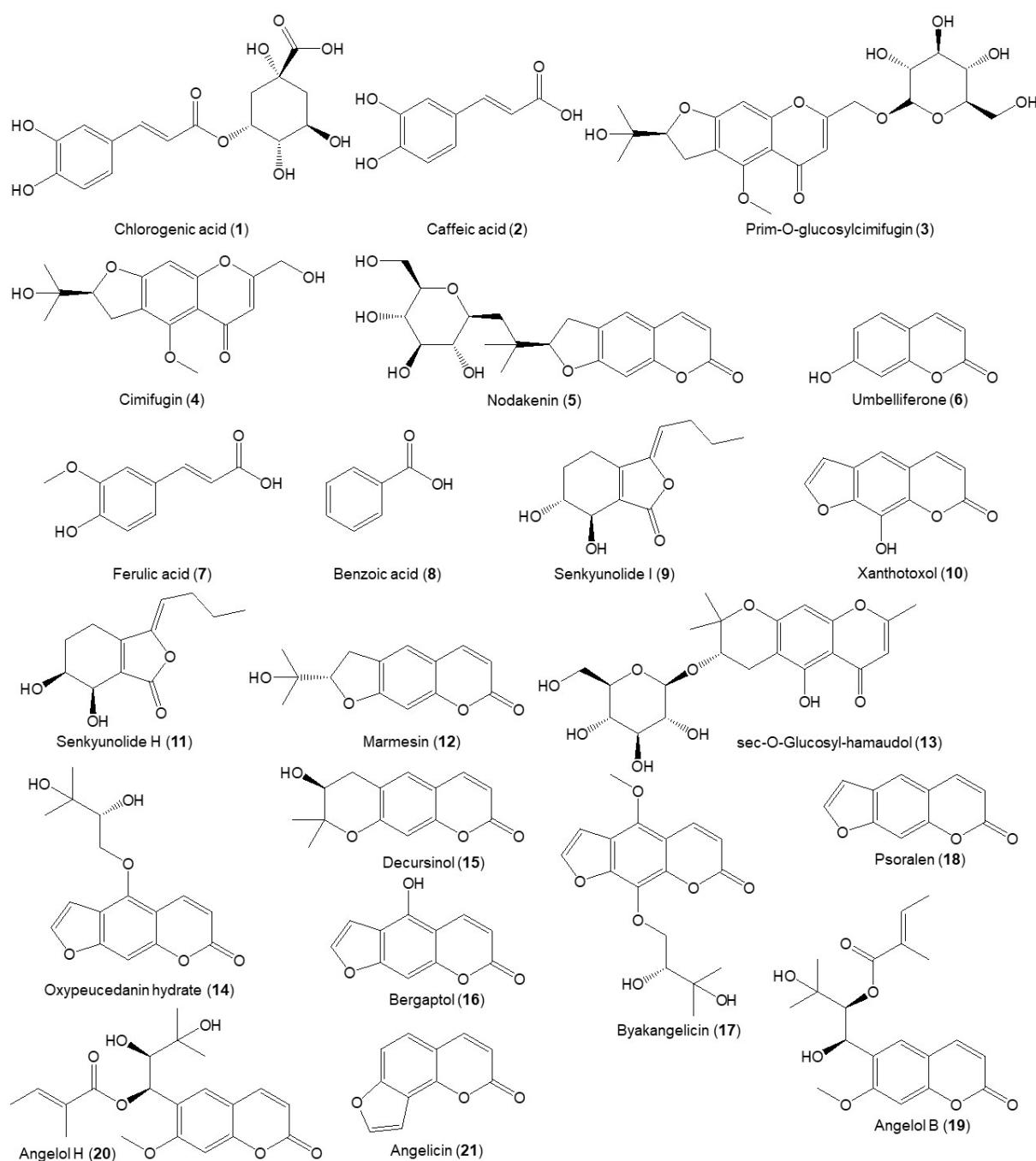
Continued.



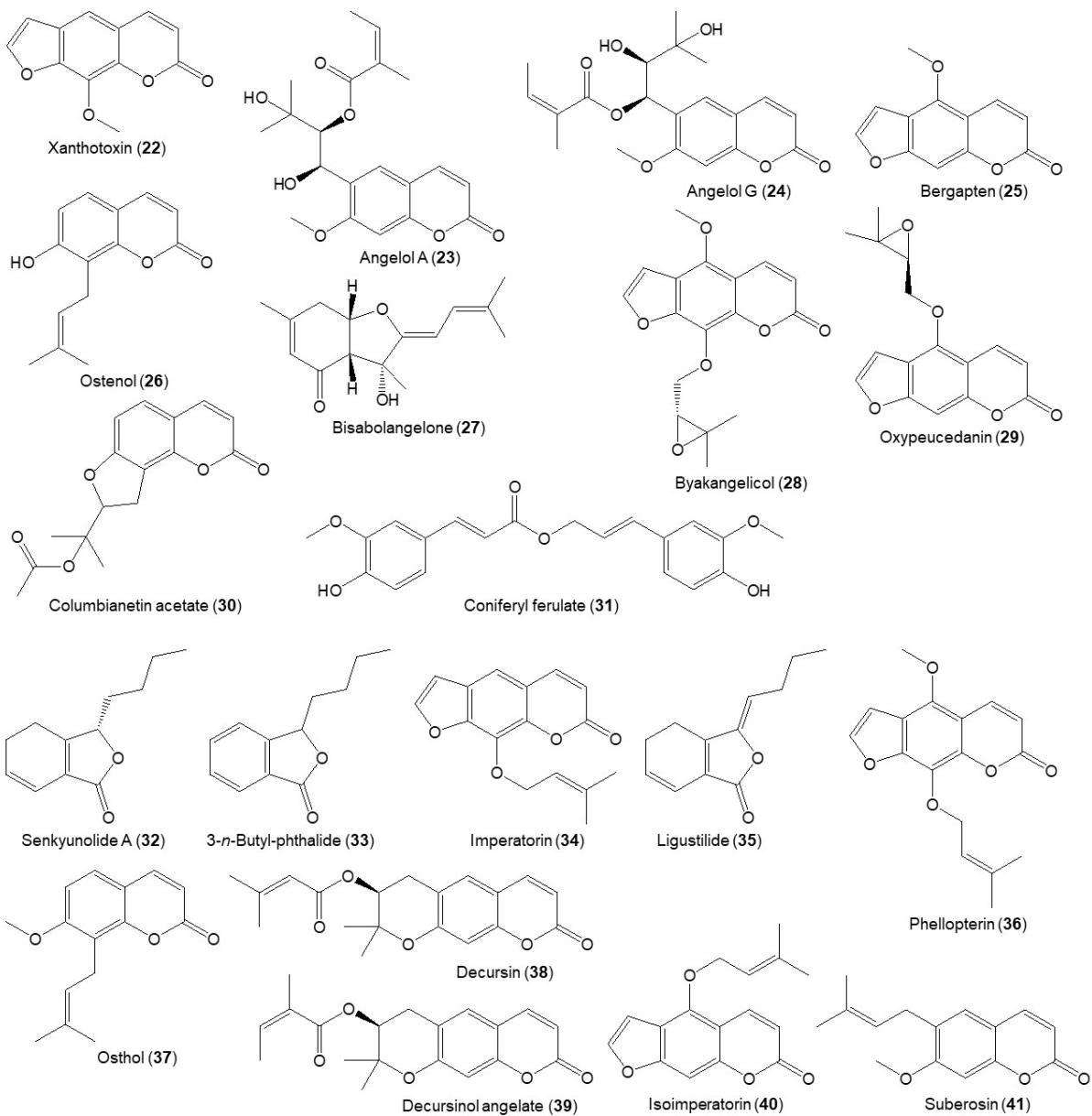
Continued.



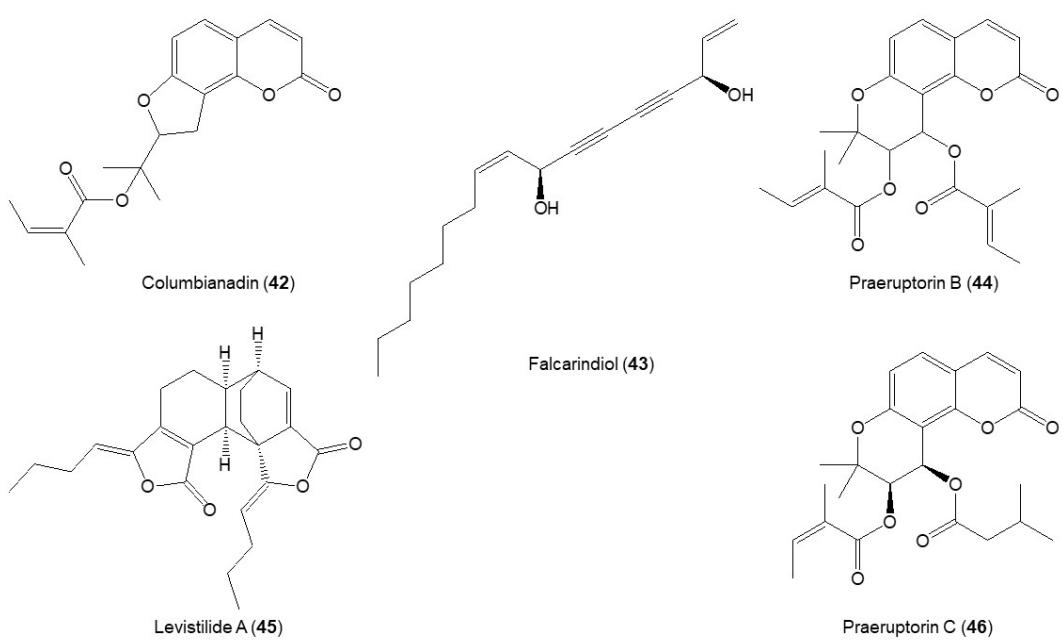
Continued.



**Figure S5.** Chemical structures of 46 marker compounds.



Continued.



Continued.

**Table S1.** The sequence identity matrix and sequence difference count matrix of ITS nucleotide sequences in Table 1.

| Matrix                           | Seq-> | ABI   | ADA   | ASI   | AGI   | AAC   | ADE   | ARE   | APO   | CTE   | OGR   |
|----------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Sequence identity matrix         | ABI   | ID    | 0.962 | 0.895 | 0.972 | 0.973 | 0.965 | 0.972 | 0.975 | 0.914 | 0.835 |
|                                  | ADA   | 0.962 | ID    | 0.892 | 0.963 | 0.962 | 0.952 | 0.96  | 0.963 | 0.907 | 0.833 |
|                                  | ASI   | 0.895 | 0.892 | ID    | 0.904 | 0.91  | 0.894 | 0.9   | 0.898 | 0.942 | 0.846 |
|                                  | AGI   | 0.972 | 0.963 | 0.904 | ID    | 0.984 | 0.982 | 0.973 | 0.973 | 0.921 | 0.84  |
|                                  | AAC   | 0.973 | 0.962 | 0.91  | 0.984 | ID    | 0.975 | 0.978 | 0.975 | 0.926 | 0.84  |
|                                  | ADE   | 0.965 | 0.952 | 0.894 | 0.982 | 0.975 | ID    | 0.965 | 0.968 | 0.913 | 0.833 |
|                                  | ARE   | 0.972 | 0.96  | 0.9   | 0.973 | 0.978 | 0.965 | ID    | 0.975 | 0.918 | 0.832 |
|                                  | APO   | 0.975 | 0.963 | 0.898 | 0.973 | 0.975 | 0.968 | 0.975 | ID    | 0.911 | 0.833 |
|                                  | CTE   | 0.914 | 0.907 | 0.942 | 0.921 | 0.926 | 0.913 | 0.918 | 0.911 | ID    | 0.853 |
|                                  | OGR   | 0.835 | 0.833 | 0.846 | 0.84  | 0.84  | 0.833 | 0.832 | 0.833 | 0.853 | ID    |
| Matrix                           | Seq-> | ABI   | ADA   | ASI   | AGI   | AAC   | ADE   | ARE   | APO   | CTE   | OGR   |
| Sequence difference count matrix | ABI   | ID    | 26    | 72    | 19    | 18    | 24    | 19    | 17    | 59    | 115   |
|                                  | ADA   | 26    | ID    | 74    | 25    | 26    | 33    | 27    | 25    | 64    | 116   |
|                                  | ASI   | 72    | 74    | ID    | 66    | 62    | 73    | 69    | 70    | 40    | 107   |
|                                  | AGI   | 19    | 25    | 66    | ID    | 11    | 12    | 18    | 18    | 54    | 111   |
|                                  | AAC   | 18    | 26    | 62    | 11    | ID    | 17    | 15    | 17    | 51    | 111   |
|                                  | ADE   | 24    | 33    | 73    | 12    | 17    | ID    | 24    | 22    | 60    | 116   |
|                                  | ARE   | 19    | 27    | 69    | 18    | 15    | 24    | ID    | 17    | 56    | 117   |
|                                  | APO   | 17    | 25    | 70    | 18    | 17    | 22    | 17    | ID    | 61    | 116   |
|                                  | CTE   | 59    | 64    | 40    | 54    | 51    | 60    | 56    | 61    | ID    | 102   |
|                                  | OGR   | 115   | 116   | 107   | 111   | 111   | 116   | 117   | 116   | 102   | ID    |

**Table S2.** The sequence identity matrix and sequence difference count matrix of *psbA-trnH* nucleotide sequences in Table 1.

| Matrix                           | Seq-> | ABI   | ARE   | APO   | ADA   | AGI   | AAC   | ASI   | CTE   | ADE   | OGR   |
|----------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Sequence Identity Matrix         | ABI   | ID    | 0.98  | 0.926 | 0.917 | 0.94  | 0.914 | 0.851 | 0.796 | 0.937 | 0.741 |
|                                  | ARE   | 0.98  | ID    | 0.926 | 0.909 | 0.931 | 0.905 | 0.851 | 0.791 | 0.923 | 0.738 |
|                                  | APO   | 0.926 | 0.926 | ID    | 0.961 | 0.955 | 0.935 | 0.882 | 0.821 | 0.952 | 0.761 |
|                                  | ADA   | 0.917 | 0.909 | 0.961 | ID    | 0.975 | 0.954 | 0.888 | 0.832 | 0.967 | 0.765 |
|                                  | AGI   | 0.94  | 0.931 | 0.955 | 0.975 | ID    | 0.972 | 0.906 | 0.841 | 0.99  | 0.779 |
|                                  | AAC   | 0.914 | 0.905 | 0.935 | 0.954 | 0.972 | ID    | 0.92  | 0.852 | 0.963 | 0.789 |
|                                  | ASI   | 0.851 | 0.851 | 0.882 | 0.888 | 0.906 | 0.92  | ID    | 0.917 | 0.909 | 0.847 |
|                                  | CTE   | 0.796 | 0.791 | 0.821 | 0.832 | 0.841 | 0.852 | 0.917 | ID    | 0.843 | 0.876 |
|                                  | ADE   | 0.937 | 0.923 | 0.952 | 0.967 | 0.99  | 0.963 | 0.909 | 0.843 | ID    | 0.784 |
|                                  | OGR   | 0.741 | 0.738 | 0.761 | 0.765 | 0.779 | 0.789 | 0.847 | 0.876 | 0.784 | ID    |
| Matrix                           | Seq-> | ABI   | ARE   | APO   | ADA   | AGI   | AAC   | ASI   | CTE   | ADE   | OGR   |
| Sequence difference count Matrix | ABI   | ID    | 7     | 26    | 29    | 21    | 30    | 52    | 73    | 22    | 94    |
|                                  | ARE   | 7     | ID    | 26    | 32    | 24    | 33    | 52    | 75    | 27    | 95    |
|                                  | APO   | 26    | 26    | ID    | 13    | 15    | 22    | 40    | 62    | 16    | 84    |
|                                  | ADA   | 29    | 32    | 13    | ID    | 8     | 15    | 37    | 57    | 11    | 81    |
|                                  | AGI   | 21    | 24    | 15    | 8     | ID    | 9     | 31    | 54    | 3     | 76    |
|                                  | AAC   | 30    | 33    | 22    | 15    | 9     | ID    | 26    | 49    | 12    | 71    |
|                                  | ASI   | 52    | 52    | 40    | 37    | 31    | 26    | ID    | 26    | 30    | 49    |
|                                  | CTE   | 73    | 75    | 62    | 57    | 54    | 49    | 26    | ID    | 53    | 39    |
|                                  | ADE   | 22    | 27    | 16    | 11    | 3     | 12    | 30    | 53    | ID    | 74    |
|                                  | OGR   | 94    | 95    | 84    | 81    | 76    | 71    | 49    | 39    | 74    | ID    |

**Table S3.** Regression equation, linear range, correlation coefficient, limit of detection, and limit of quantification of the marker compounds

| Compound                               | UV (nm) | t <sub>R</sub> (min) | Regression equation    | Linear range (µg/mL) | r <sup>2</sup> | LOD (µg/mL) | LOQ (µg/mL) |
|--|---------|----------------------|------------------------|----------------------|----------------|-------------|-------------|
| Chlorogenic acid ( <b>1</b> )          | 325nm   | 6.33                 | y = 18.9882x - 20.1736 | 4.69–300.00          | 1.0000         | 0.04        | 0.14        |
| Caffeic acid ( <b>2</b> )              | 325nm   | 8.83                 | y = 35.6640x - 3.0620  | 0.08–5.00            | 0.9992         | 0.02        | 0.07        |
| Prim-O-glucosyl-cimifugin ( <b>3</b> ) | 230nm   | 9.56                 | y = 18.3489x - 0.9000  | 1.56–100.00          | 1.0000         | 0.03        | 0.11        |
| Cimifugin ( <b>4</b> )                 | 230nm   | 13.06                | y = 26.7282x - 1.3057  | 0.78–50.00           | 1.0000         | 0.02        | 0.08        |
| Nodakenin ( <b>5</b> )                 | 325nm   | 13.27                | y = 18.8847x - 0.5929  | 0.78–50.00           | 1.0000         | 0.02        | 0.07        |
| Umbelliferone ( <b>6</b> )             | 325nm   | 13.44                | y = 14.3679x - 2.3615  | 1.56–100.00          | 1.0000         | 0.01        | 0.03        |
| Ferulic acid ( <b>7</b> )              | 325nm   | 13.55                | y = 39.8067x + 5.0408  | 0.70–45.00           | 1.0000         | 0.01        | 0.04        |
| Benzoic acid ( <b>8</b> )              | 230nm   | 16.64                | y = 45.7381x + 0.3989  | 0.08–5.00            | 1.0000         | 0.01        | 0.03        |
| Senkyunolide I ( <b>9</b> )            | 280nm   | 17.67                | y = 37.2178x + 3.1287  | 0.78–50.00           | 1.0000         | 0.02        | 0.05        |
| Xanthotoxol ( <b>10</b> )              | 250nm   | 18.05                | y = 44.2476x + 0.0661  | 0.16–10.00           | 1.0000         | 0.01        | 0.04        |
| Senkyunolide H ( <b>11</b> )           | 280nm   | 18.74                | y = 41.3349x + 0.9230  | 0.16–10.00           | 1.0000         | 0.02        | 0.05        |
| Marmesin ( <b>12</b> )                 | 325nm   | 19.53                | y = 35.2619x - 1.3776  | 0.78–50.00           | 1.0000         | 0.01        | 0.04        |
| sec-O-Glucosyl-hamaudol ( <b>13</b> )  | 250nm   | 19.85                | y = 15.3224x - 0.0649  | 0.16–10.00           | 1.0000         | 0.02        | 0.06        |
| Oxypeucedanin hydrate ( <b>14</b> )    | 250nm   | 20.68                | y = 34.9383x - 0.7443  | 2.34–150.00          | 1.0000         | 0.01        | 0.05        |
| Decursinol ( <b>15</b> )               | 325nm   | 20.77                | y = 28.3230x - 0.2477  | 0.16–10.00           | 1.0000         | 0.01        | 0.05        |
| Bergaptol ( <b>16</b> )                | 270nm   | 21.46                | y = 20.9488x + 1.4414  | 0.78–50.00           | 1.0000         | 0.02        | 0.07        |
| Byakangelicin ( <b>17</b> )            | 270nm   | 21.38                | y = 28.2776x + 1.4902  | 3.13–200.00          | 1.0000         | 0.02        | 0.06        |
| Psoralen ( <b>18</b> )                 | 250nm   | 25.07                | y = 67.6458x - 0.3091  | 0.08–5.00            | 0.9999         | 0.01        | 0.03        |
| Angelol B ( <b>19</b> )                | 325nm   | 25.56                | y = 15.2751x + 2.9632  | 1.56–100.00          | 0.9999         | 0.04        | 0.13        |
| Angelol H ( <b>20</b> )                | 325nm   | 25.72                | y = 18.7174x + 1.5684  | 0.78–50.00           | 0.9999         | 0.03        | 0.10        |
| Angelicin ( <b>21</b> )                | 250nm   | 26.04                | y = 62.3088x + 1.2799  | 0.16–10.00           | 1.0000         | 0.01        | 0.03        |
| Xanthotoxin ( <b>22</b> )              | 250nm   | 26.25                | y = 55.4055x - 0.7218  | 0.16–10.00           | 1.0000         | 0.01        | 0.04        |
| Angelol A ( <b>23</b> )                | 325nm   | 26.72                | y = 14.9625x + 0.1126  | 0.16–10.00           | 1.0000         | 0.03        | 0.11        |
| Angelol G ( <b>24</b> )                | 325nm   | 27.88                | y = 20.3961x + 7.2678  | 2.34–150.00          | 0.9999         | 0.03        | 0.09        |
| Bergapten ( <b>25</b> )                | 250nm   | 29.07                | y = 46.7556x - 1.1437  | 0.16–10.00           | 1.0000         | 0.01        | 0.05        |

|                                     |       |       |                          |             |        |      |      |
|-------------------------------------|-------|-------|--------------------------|-------------|--------|------|------|
| Ostenol ( <b>26</b> )               | 325nm | 30.99 | $y = 21.7660x + 0.1259$  | 0.16–10.00  | 1.0000 | 0.02 | 0.06 |
| Bisabolangelone ( <b>27</b> )       | 250nm | 31.99 | $y = 22.5984x + 0.2770$  | 1.56–100.00 | 1.0000 | 0.02 | 0.08 |
| Byakangelicol ( <b>28</b> )         | 270nm | 32.84 | $y = 19.7989x - 0.0385$  | 0.31–20.00  | 1.0000 | 0.03 | 0.10 |
| Oxypeucedanin ( <b>29</b> )         | 250nm | 33.16 | $y = 27.5815x + 1.9420$  | 1.56–100.00 | 1.0000 | 0.02 | 0.08 |
| Columbianetin acetate ( <b>30</b> ) | 325nm | 33.28 | $y = 25.8919x + 7.4690$  | 1.56–100.00 | 0.9999 | 0.02 | 0.08 |
| Coniferyl ferulate ( <b>31</b> )    | 325nm | 33.58 | $y = 5.6940x - 2.5937$   | 0.78–50.00  | 1.0000 | 0.11 | 0.37 |
| Senkyunolide A ( <b>32</b> )        | 280nm | 36.53 | $y = 5.4381x + 0.7766$   | 0.47–30.00  | 0.9999 | 0.08 | 0.26 |
| 3-n-Butyl-phthalide ( <b>33</b> )   | 230nm | 37.72 | $y = 22.6709x - 0.4780$  | 0.16–10.00  | 1.0000 | 0.03 | 0.09 |
| Imperatorin ( <b>34</b> )           | 250nm | 40.49 | $y = 49.3342x + 4.3161$  | 0.08–5.00   | 1.0000 | 0.01 | 0.03 |
| Ligustilide ( <b>35</b> )           | 325nm | 42.41 | $y = 12.6081x + 7.9914$  | 4.69–300.00 | 1.0000 | 0.06 | 0.20 |
| Phellopterin ( <b>36</b> )          | 270nm | 42.68 | $y = 31.7581x + 1.6885$  | 3.13–200.00 | 1.0000 | 0.02 | 0.07 |
| Osthol ( <b>37</b> )                | 325nm | 43.19 | $y = 31.7406x + 24.8006$ | 3.91–250.00 | 0.9999 | 0.02 | 0.08 |
| Decursin ( <b>38</b> )              | 325nm | 43.94 | $y = 30.1186x - 3.7925$  | 6.25–400.00 | 1.0000 | 0.02 | 0.06 |
| Decursinol angelate ( <b>39</b> )   | 325nm | 44.40 | $y = 19.4719x - 3.6483$  | 6.25–400.00 | 1.0000 | 0.03 | 0.09 |
| Isoimperatorin ( <b>40</b> )        | 250nm | 44.73 | $y = 33.7227x + 2.9736$  | 2.34–150.00 | 1.0000 | 0.02 | 0.07 |
| Suberosin ( <b>41</b> )             | 325nm | 45.75 | $y = 26.4464x - 0.2940$  | 0.08–5.00   | 1.0000 | 0.02 | 0.07 |
| Columbianadin ( <b>42</b> )         | 325nm | 46.02 | $y = 25.1184x + 6.8247$  | 1.56–100.00 | 0.9999 | 0.03 | 0.09 |
| Falcarindiol ( <b>43</b> )          | 250nm | 48.58 | $y = 0.9440x + 0.0718$   | 2.34–150.00 | 1.0000 | 0.62 | 2.07 |
| Praeruptorin B ( <b>44</b> )        | 325nm | 55.60 | $y = 17.2871x + 2.1391$  | 1.25–80.00  | 1.0000 | 0.04 | 0.14 |
| Levistilide A ( <b>45</b> )         | 280nm | 55.79 | $y = 13.5757x + 1.0816$  | 1.56–100.00 | 1.0000 | 0.06 | 0.21 |
| Praeruptorin C ( <b>46</b> )        | 325nm | 57.84 | $y = 17.1114x + 0.4494$  | 0.16–10.00  | 0.9999 | 0.04 | 0.14 |

tR, retention time; UV, detection wavelength;  $r^2$ , correlation coefficient; LOD, limit of detection; LOQ, limit of quantification.

**Table S4.** Intra- and interday precisions of the marker compounds

| Compound                               | Initial conc. ( $\mu\text{g/mL}$ ) | Intraday ( $n = 3$ )                |         |              | Interday ( $n = 3$ )                |         |              |
|--|------------------------------------|-------------------------------------|---------|--------------|-------------------------------------|---------|--------------|
|  |                                    | Detected conc. ( $\mu\text{g/mL}$ ) | RSD (%) | Accuracy (%) | Detected conc. ( $\mu\text{g/mL}$ ) | RSD (%) | Accuracy (%) |
| Chlorogenic acid ( <b>1</b> )          | 37.50                              | 36.76                               | 0.20    | 98.04        | 36.98                               | 0.95    | 98.60        |
|  | 150.00                             | 145.73                              | 0.07    | 97.15        | 146.87                              | 1.38    | 97.91        |
| Caffeic acid ( <b>2</b> )              | 0.63                               | 0.58                                | 0.84    | 92.25        | 0.58                                | 1.11    | 93.29        |
|  | 2.50                               | 2.42                                | 0.48    | 96.60        | 2.43                                | 0.87    | 97.35        |
| Prim-O-glucosyl-cimifugin ( <b>3</b> ) | 12.50                              | 12.53                               | 0.40    | 100.21       | 12.53                               | 0.31    | 100.26       |
|  | 50.00                              | 50.57                               | 1.60    | 101.14       | 50.56                               | 1.62    | 101.13       |
| Cimifugin ( <b>4</b> )                 | 6.25                               | 6.29                                | 0.30    | 100.57       | 6.28                                | 0.31    | 100.53       |
|  | 25.00                              | 25.28                               | 1.43    | 101.13       | 25.26                               | 1.57    | 101.05       |
| Nodakenin ( <b>5</b> )                 | 6.25                               | 6.23                                | 0.54    | 99.66        | 6.26                                | 0.39    | 100.20       |
|  | 25.00                              | 24.42                               | 0.09    | 97.66        | 24.57                               | 1.01    | 98.28        |
| Umbelliferone ( <b>6</b> )             | 12.50                              | 12.61                               | 0.25    | 100.89       | 12.59                               | 0.58    | 100.68       |
|  | 50.00                              | 50.48                               | 1.36    | 100.95       | 50.43                               | 1.53    | 100.85       |
| Ferulic acid ( <b>7</b> )              | 5.63                               | 5.66                                | 0.09    | 100.65       | 5.67                                | 0.21    | 100.72       |
|  | 22.50                              | 22.06                               | 0.22    | 98.05        | 22.21                               | 1.40    | 98.73        |
| Benzoic acid ( <b>8</b> )              | 0.63                               | 0.63                                | 0.72    | 101.22       | 0.63                                | 1.03    | 101.45       |
|  | 2.50                               | 2.48                                | 0.84    | 99.03        | 2.49                                | 0.46    | 99.52        |
| Senkyunolide I ( <b>9</b> )            | 6.25                               | 6.29                                | 0.07    | 100.66       | 6.29                                | 0.09    | 100.68       |
|  | 25.00                              | 24.51                               | 0.20    | 98.03        | 24.64                               | 1.16    | 98.57        |
| Xanthotoxol ( <b>10</b> )              | 1.25                               | 1.27                                | 0.78    | 101.49       | 1.26                                | 1.17    | 101.13       |
|  | 5.00                               | 5.03                                | 0.82    | 100.68       | 5.03                                | 0.84    | 100.66       |
| Senkyunolide H ( <b>11</b> )           | 1.25                               | 1.26                                | 0.22    | 100.66       | 1.26                                | 0.22    | 100.66       |
|  | 5.00                               | 4.92                                | 0.16    | 98.32        | 4.94                                | 1.14    | 98.89        |
| Marmesin ( <b>12</b> )                 | 6.25                               | 6.30                                | 0.12    | 100.72       | 6.29                                | 0.20    | 100.60       |
|  | 25.00                              | 24.49                               | 0.01    | 97.95        | 24.60                               | 0.84    | 98.42        |

|                                       |        |        |      |        |        |      |        |
|---------------------------------------|--------|--------|------|--------|--------|------|--------|
| sec-O-Glucosyl-hamaudol ( <b>13</b> ) | 1.25   | 1.24   | 0.30 | 98.84  | 1.24   | 1.09 | 99.37  |
|                                       | 5.00   | 4.97   | 1.25 | 99.42  | 4.99   | 0.69 | 99.81  |
| Oxypeucedanin hydrate ( <b>14</b> )   | 18.75  | 18.95  | 0.55 | 101.07 | 18.85  | 1.22 | 100.54 |
|                                       | 75.00  | 75.57  | 0.81 | 100.77 | 75.62  | 0.71 | 100.83 |
| Decursinol ( <b>15</b> )              | 1.25   | 1.26   | 0.32 | 100.50 | 1.26   | 0.32 | 100.50 |
|                                       | 5.00   | 4.90   | 0.04 | 98.00  | 4.92   | 0.83 | 98.45  |
| Bergaptol ( <b>16</b> )               | 6.25   | 6.22   | 0.12 | 99.51  | 6.24   | 0.69 | 99.84  |
|                                       | 25.00  | 24.85  | 0.12 | 99.42  | 24.92  | 0.58 | 99.69  |
| Byakangelicin ( <b>17</b> )           | 25.00  | 25.31  | 0.52 | 101.26 | 25.18  | 1.18 | 100.73 |
|                                       | 100.00 | 100.69 | 0.80 | 100.69 | 100.75 | 0.68 | 100.75 |
| Psoralen ( <b>18</b> )                | 0.63   | 0.63   | 0.36 | 100.39 | 0.63   | 0.36 | 100.39 |
|                                       | 2.50   | 2.45   | 0.14 | 98.12  | 2.46   | 0.80 | 98.50  |
| Angelol B ( <b>19</b> )               | 12.50  | 12.66  | 0.06 | 101.27 | 12.66  | 0.09 | 101.26 |
|                                       | 50.00  | 50.24  | 0.08 | 100.49 | 50.30  | 0.26 | 100.60 |
| Angelol H ( <b>20</b> )               | 6.25   | 6.36   | 0.13 | 101.72 | 6.36   | 0.21 | 101.81 |
|                                       | 25.00  | 25.12  | 0.26 | 100.48 | 25.14  | 0.15 | 100.58 |
| Angelicin ( <b>21</b> )               | 1.25   | 1.26   | 0.07 | 100.77 | 1.26   | 0.22 | 100.69 |
|                                       | 5.00   | 5.05   | 0.05 | 100.91 | 5.04   | 0.16 | 100.85 |
| Xanthotoxin ( <b>22</b> )             | 1.25   | 1.26   | 0.08 | 100.77 | 1.26   | 0.14 | 100.67 |
|                                       | 5.00   | 4.90   | 0.11 | 98.10  | 4.93   | 0.70 | 98.55  |
| Angelol A ( <b>23</b> )               | 1.25   | 1.27   | 1.05 | 101.52 | 1.26   | 1.40 | 100.99 |
|                                       | 5.00   | 5.04   | 0.69 | 100.77 | 5.04   | 0.61 | 100.81 |
| Angelol G ( <b>24</b> )               | 18.75  | 18.93  | 0.26 | 100.94 | 18.96  | 0.15 | 101.12 |
|                                       | 75.00  | 75.30  | 0.06 | 100.40 | 75.40  | 0.27 | 100.54 |
| Bergapten ( <b>25</b> )               | 1.25   | 1.25   | 0.26 | 100.40 | 1.25   | 0.17 | 100.17 |
|                                       | 5.00   | 4.90   | 0.04 | 98.02  | 4.92   | 0.72 | 98.45  |
| Ostenol ( <b>26</b> )                 | 1.25   | 1.27   | 0.63 | 101.71 | 1.27   | 1.28 | 101.22 |

|                                     |        |        |      |        |        |      |        |
|-------------------------------------|--------|--------|------|--------|--------|------|--------|
|                                     | 5.00   | 5.04   | 0.85 | 100.84 | 5.04   | 0.85 | 100.84 |
| Bisabolangelone ( <b>27</b> )       | 12.50  | 12.54  | 0.07 | 100.35 | 12.55  | 0.16 | 100.40 |
|                                     | 50.00  | 50.12  | 0.04 | 100.23 | 50.17  | 0.23 | 100.35 |
| Byakangelicol ( <b>28</b> )         | 2.50   | 2.54   | 0.57 | 101.43 | 2.52   | 1.21 | 100.96 |
|                                     | 10.00  | 10.06  | 0.70 | 100.63 | 10.06  | 0.76 | 100.60 |
| Oxypeucedanin ( <b>29</b> )         | 12.50  | 12.72  | 0.48 | 101.73 | 12.65  | 1.17 | 101.21 |
|                                     | 50.00  | 50.46  | 0.73 | 100.92 | 50.45  | 0.78 | 100.90 |
| Columbianetin acetate ( <b>30</b> ) | 12.50  | 12.61  | 0.02 | 100.91 | 12.61  | 0.02 | 100.91 |
|                                     | 50.00  | 50.32  | 0.03 | 100.64 | 50.34  | 0.09 | 100.69 |
| Coniferyl ferulate ( <b>31</b> )    | 6.25   | 5.76   | 0.91 | 92.15  | 5.92   | 3.88 | 94.68  |
|                                     | 25.00  | 22.48  | 0.90 | 89.91  | 23.35  | 5.73 | 93.38  |
| Senkyunolide A ( <b>32</b> )        | 3.75   | 3.66   | 0.29 | 97.53  | 3.66   | 0.50 | 97.70  |
|                                     | 15.00  | 14.73  | 0.31 | 98.18  | 14.81  | 1.20 | 98.72  |
| 3-n-Butyl-phthalide ( <b>33</b> )   | 1.25   | 1.26   | 1.23 | 100.73 | 1.25   | 0.70 | 100.14 |
|                                     | 5.00   | 4.94   | 0.40 | 98.76  | 4.96   | 1.13 | 99.20  |
| Imperatorin ( <b>34</b> )           | 0.63   | 0.63   | 0.67 | 101.35 | 0.63   | 0.85 | 101.14 |
|                                     | 2.50   | 2.45   | 0.13 | 98.07  | 2.46   | 0.65 | 98.42  |
| Ligustilide ( <b>35</b> )           | 37.50  | 37.71  | 0.04 | 100.55 | 37.70  | 0.02 | 100.54 |
|                                     | 150.00 | 147.98 | 0.11 | 98.66  | 148.72 | 0.96 | 99.14  |
| Phellopterin ( <b>36</b> )          | 25.00  | 25.38  | 0.50 | 101.54 | 25.26  | 1.13 | 101.05 |
|                                     | 100.00 | 100.90 | 0.79 | 100.90 | 100.86 | 0.85 | 100.86 |
| Osthol ( <b>37</b> )                | 31.25  | 31.56  | 0.04 | 101.00 | 31.56  | 0.06 | 100.98 |
|                                     | 125.00 | 125.98 | 0.03 | 100.78 | 126.02 | 0.03 | 100.82 |
| Decursin ( <b>38</b> )              | 50.00  | 50.25  | 0.06 | 100.51 | 50.20  | 0.14 | 100.41 |
|                                     | 200.00 | 196.41 | 0.01 | 98.21  | 197.38 | 0.85 | 98.69  |
| Decursinol angelate ( <b>39</b> )   | 50.00  | 50.26  | 0.06 | 100.53 | 50.21  | 0.15 | 100.43 |
|                                     | 200.00 | 196.29 | 0.02 | 98.15  | 197.24 | 0.84 | 98.62  |

|                              |       |       |      |        |       |      |        |
|------------------------------|-------|-------|------|--------|-------|------|--------|
| Isoimperatorin ( <b>40</b> ) | 18.75 | 19.05 | 0.50 | 101.60 | 18.96 | 1.13 | 101.12 |
|                              | 75.00 | 75.67 | 0.81 | 100.90 | 75.68 | 0.79 | 100.91 |
| Suberosin ( <b>41</b> )      | 0.63  | 0.61  | 0.36 | 97.57  | 0.61  | 0.95 | 97.17  |
|                              | 2.50  | 2.47  | 0.15 | 98.61  | 2.48  | 0.75 | 99.11  |
| Columbianadin ( <b>42</b> )  | 12.50 | 12.60 | 0.00 | 100.83 | 12.60 | 0.02 | 100.82 |
|                              | 50.00 | 50.29 | 0.14 | 100.58 | 50.32 | 0.21 | 100.64 |
| Falcarindiol ( <b>43</b> )   | 18.75 | 18.85 | 0.32 | 100.54 | 18.85 | 0.32 | 100.54 |
|                              | 75.00 | 73.69 | 0.08 | 98.25  | 74.08 | 0.99 | 98.77  |
| Praeruptorin B ( <b>44</b> ) | 10.00 | 10.10 | 0.03 | 101.00 | 10.10 | 0.03 | 101.02 |
|                              | 40.00 | 39.85 | 0.04 | 99.64  | 39.90 | 0.19 | 99.74  |
| Levistilide A ( <b>45</b> )  | 12.50 | 12.56 | 0.44 | 100.50 | 12.59 | 0.43 | 100.68 |
|                              | 50.00 | 49.11 | 0.18 | 98.22  | 49.39 | 1.16 | 98.78  |
| Praeruptorin C ( <b>46</b> ) | 1.25  | 1.27  | 0.46 | 101.22 | 1.27  | 0.27 | 101.53 |
|                              | 5.00  | 5.03  | 0.07 | 100.54 | 5.03  | 0.13 | 100.65 |

Conc., concentration; RSD, relative standard deviation.

**Table S5.** Recoveries of the marker compounds (*n* = 3)

| Compound                               | Initial conc.<br>( $\mu\text{g/mL}$ ) | Spiked conc.<br>( $\mu\text{g/mL}$ ) | Detected conc.<br>( $\mu\text{g/mL}$ ) | Recovery (%) | RSD(%) |
|--|---------------------------------------|--------------------------------------|--|--------------|--------|
| Chlorogenic acid ( <b>1</b> )          | 32.17                                 | 37.50                                | 73.32                                  | 109.72       | 1.57   |
|  |                                       | 150.00                               | 196.10                                 | 109.28       | 2.58   |
| Caffeic acid ( <b>2</b> )              | 0.52                                  | 1.00                                 | 1.45                                   | 92.72        | 1.40   |
|  |                                       | 4.00                                 | 4.46                                   | 98.63        | 0.93   |
| Prim-O-glucosyl-cimifugin ( <b>3</b> ) | 20.19                                 | 6.25                                 | 27.06                                  | 109.93       | 8.22   |
|  |                                       | 25.00                                | 47.73                                  | 110.15       | 6.06   |
| Cimifugin ( <b>4</b> )                 | 7.46                                  | 3.13                                 | 10.82                                  | 107.63       | 8.01   |
|  |                                       | 12.50                                | 21.35                                  | 111.13       | 3.34   |
| Nodakenin ( <b>5</b> )                 | 147.18                                | 20.00                                | 168.91                                 | 108.68       | 5.51   |
|  |                                       | 80.00                                | 232.10                                 | 106.16       | 4.52   |
| Umbelliferone ( <b>6</b> )             | 9.33                                  | 4.40                                 | 13.70                                  | 99.34        | 4.15   |
|  |                                       | 17.50                                | 27.44                                  | 103.48       | 0.34   |
| Ferulic acid ( <b>7</b> )              | 6.93                                  | 5.63                                 | 13.10                                  | 109.77       | 1.51   |
|  |                                       | 22.50                                | 31.58                                  | 109.55       | 1.31   |
| Benzoic acid ( <b>8</b> )              | 0.47                                  | 0.63                                 | 1.14                                   | 107.86       | 1.14   |
|  |                                       | 2.50                                 | 3.11                                   | 105.56       | 2.30   |
| Senkyunolide I ( <b>9</b> )            | 9.92                                  | 6.25                                 | 16.78                                  | 109.77       | 2.34   |
|  |                                       | 25.00                                | 37.16                                  | 108.96       | 1.07   |
| Xanthotoxol ( <b>10</b> )              | 0.79                                  | 0.63                                 | 1.45                                   | 105.59       | 2.47   |
|  |                                       | 2.50                                 | 3.42                                   | 105.35       | 1.15   |
| Senkyunolide H ( <b>11</b> )           | 1.99                                  | 1.25                                 | 3.35                                   | 109.03       | 3.87   |
|  |                                       | 5.00                                 | 7.40                                   | 108.30       | 0.75   |
| Marmesin ( <b>12</b> )                 | 5.72                                  | 6.25                                 | 12.10                                  | 102.08       | 2.16   |
|  |                                       | 25.00                                | 31.47                                  | 103.02       | 0.92   |
| sec-O-Glucosyl-hamaudol ( <b>13</b> )  | 1.57                                  | 0.63                                 | 2.26                                   | 109.64       | 6.67   |
|  |                                       | 2.50                                 | 4.34                                   | 110.69       | 1.31   |
| Oxypeucedanin hydrate ( <b>14</b> )    | 15.14                                 | 9.38                                 | 24.91                                  | 104.13       | 2.28   |
|  |                                       | 37.50                                | 55.56                                  | 107.79       | 1.05   |
| Decursinol ( <b>15</b> )               | 5.46                                  | 1.25                                 | 6.71                                   | 100.18       | 3.21   |
|  |                                       | 5.00                                 | 10.55                                  | 101.73       | 1.71   |
| Bergaptol ( <b>16</b> )                | 3.68                                  | 3.13                                 | 6.95                                   | 104.48       | 3.55   |
|  |                                       | 12.50                                | 17.05                                  | 106.93       | 0.78   |
| Byakangelicin ( <b>17</b> )            | 13.69                                 | 12.50                                | 26.90                                  | 105.73       | 1.85   |
|  |                                       | 50.00                                | 67.77                                  | 108.16       | 0.94   |
| Psoralen ( <b>18</b> )                 | 0.61                                  | 0.63                                 | 1.25                                   | 102.10       | 1.51   |
|  |                                       | 2.50                                 | 3.17                                   | 102.49       | 0.81   |
| Angelol B ( <b>19</b> )                | 39.38                                 | 6.25                                 | 45.63                                  | 99.86        | 5.71   |
|  |                                       | 25.00                                | 66.52                                  | 108.53       | 4.37   |
| Angelol H ( <b>20</b> )                | 14.66                                 | 3.13                                 | 17.62                                  | 94.88        | 7.23   |

|  |        |                 |                  |                  |              |
|--|--------|-----------------|------------------|------------------|--------------|
|  |        | 12.50           | 26.99            | 98.63            | 3.60         |
| Angelicin ( <b>21</b> )                    | 0.60   | 0.63<br>2.50    | 1.29<br>3.30     | 110.25<br>107.81 | 0.94<br>3.93 |
| Xanthotoxin ( <b>22</b> )                  | 3.03   | 1.25<br>5.00    | 4.29<br>8.14     | 100.88<br>102.14 | 3.31<br>1.39 |
| Angelol A ( <b>23</b> )                    | 0.36   | 0.63<br>2.50    | 1.01<br>3.04     | 104.44<br>107.38 | 1.56<br>0.80 |
| Angelol G ( <b>24</b> )                    | 54.40  | 9.38<br>37.50   | 63.42<br>93.71   | 96.24<br>104.84  | 8.54<br>5.87 |
| Bergapten ( <b>25</b> )                    | 1.68   | 1.25<br>5.00    | 2.94<br>6.80     | 101.18<br>102.35 | 2.79<br>0.98 |
| Ostenol ( <b>26</b> )                      | 0.06   | 0.63<br>2.50    | 0.72<br>2.74     | 105.12<br>107.32 | 2.10<br>0.91 |
| Bisabolangelone ( <b>27</b> )              | 6.21   | 6.25<br>25.00   | 12.98<br>33.25   | 108.33<br>108.15 | 1.22<br>1.01 |
| Byakangelicol ( <b>28</b> )                | 2.02   | 1.25<br>5.00    | 3.30<br>7.33     | 102.36<br>106.13 | 3.01<br>0.55 |
| Oxypeucedanin ( <b>29</b> )                | 10.14  | 6.25<br>25.00   | 16.70<br>37.35   | 104.86<br>108.81 | 3.31<br>0.64 |
| Columbianetin acetate ( <b>30</b> )        | 10.43  | 6.25<br>25.00   | 17.17<br>37.61   | 107.87<br>108.74 | 1.42<br>1.50 |
| Coniferyl ferulate ( <b>31</b> )           | 1.80   | 1.00<br>4.00    | 2.84<br>6.12     | 104.50<br>107.94 | 3.03<br>2.16 |
| Senkyunolide A ( <b>32</b> )               | 3.76   | 3.75<br>15.00   | 7.68<br>19.85    | 104.45<br>107.23 | 1.63<br>2.97 |
| 3- <i>n</i> -Butyl-phthalide ( <b>33</b> ) | 0.93   | 1.25<br>5.00    | 2.19<br>6.12     | 100.80<br>103.72 | 4.77<br>1.26 |
| Imperatorin ( <b>34</b> )                  | 0.14   | 0.63<br>2.50    | 0.76<br>2.70     | 99.13<br>102.35  | 0.68<br>0.48 |
| Ligustilide ( <b>35</b> )                  | 67.32  | 37.50<br>150.00 | 108.48<br>229.76 | 109.75<br>108.29 | 2.64<br>1.01 |
| Phellopterin ( <b>36</b> )                 | 16.36  | 12.50<br>50.00  | 29.58<br>70.72   | 105.81<br>108.72 | 2.98<br>0.59 |
| Osthol ( <b>37</b> )                       | 80.79  | 15.63<br>62.50  | 96.75<br>148.47  | 102.13<br>108.28 | 1.62<br>2.71 |
| Decursin ( <b>38</b> )                     | 495.60 | 50.00<br>200.00 | 548.89<br>701.51 | 106.58<br>102.95 | 6.86<br>6.29 |
| Decursinol angelate ( <b>39</b> )          | 471.55 | 50.00<br>200.00 | 523.77<br>678.01 | 104.43<br>103.23 | 4.61<br>6.44 |
| Isoimperatorin ( <b>40</b> )               | 10.41  | 9.38<br>37.50   | 20.20<br>50.91   | 104.49<br>108.00 | 1.89<br>0.69 |

|                              |       |       |        |        |      |
|------------------------------|-------|-------|--------|--------|------|
| Suberosin ( <b>41</b> )      | 0.57  | 0.63  | 1.19   | 99.32  | 2.44 |
|                              |       | 2.50  | 3.18   | 104.39 | 2.55 |
| Columbianadin ( <b>42</b> )  | 38.81 | 6.25  | 45.13  | 101.13 | 3.23 |
|                              |       | 25.00 | 65.66  | 107.42 | 3.17 |
| Falcarindiol ( <b>43</b> )   | 50.42 | 18.75 | 69.77  | 103.20 | 4.15 |
|                              |       | 75.00 | 131.14 | 107.63 | 0.99 |
| Praeruptorin B ( <b>44</b> ) | 19.47 | 5.00  | 24.53  | 101.08 | 2.92 |
|                              |       | 20.00 | 41.51  | 110.17 | 4.26 |
| Levistilide A ( <b>45</b> )  | 12.87 | 12.50 | 26.55  | 109.49 | 1.15 |
|                              |       | 50.00 | 66.86  | 107.99 | 1.02 |
| Praeruptorin C ( <b>46</b> ) | 3.79  | 0.63  | 4.39   | 96.12  | 6.94 |
|                              |       | 2.50  | 6.55   | 110.34 | 2.29 |

Conc., concentration; RSD, relative standard deviation.

**Table S6.** Mean amounts of the marker compounds in the methanol extracts of *Angelica acutiloba* samples (mg/g)

| Compound                          | AAC-01         | AAC-02        | AAC-03        | AAC-04        | AAC-05        | AAC-06        | AAC-07         | AAC-08        | AAC-09        | AAC-10        | AAC-11        | AAC-12        | AAC-13        |
|-----------------------------------|----------------|---------------|---------------|---------------|---------------|---------------|----------------|---------------|---------------|---------------|---------------|---------------|---------------|
| Chlorogenic acid ( <b>1</b> )     | 11.779 ± 0.382 | 4.795 ± 0.014 | 1.474 ± 0.046 | 2.892 ± 0.101 | 1.644 ± 0.059 | 4.170 ± 0.091 | 13.170 ± 0.321 | 3.284 ± 0.071 | 3.523 ± 0.044 | 6.531 ± 0.093 | 4.408 ± 0.188 | 5.059 ± 0.076 | 4.689 ± 0.241 |
| Caffeic acid ( <b>2</b> )         | 0.463 ± 0.016  | 0.074 ± 0.004 | 0.047 ± 0.003 | 0.057 ± 0.002 | 0.101 ± 0.005 | 0.220 ± 0.008 | 0.137 ± 0.009  | 0.099 ± 0.001 | 0.176 ± 0.007 | 0.087 ± 0.004 | 0.038 ± 0.003 | 0.059 ± 0.002 | -             |
| Nodakenin ( <b>5</b> )            | 28.338 ± 0.535 | -             | -             | -             | -             | 2.257 ± 0.022 | -              | -             | -             | -             | -             | -             | -             |
| Umbelliferone ( <b>6</b> )        | -              | 1.068 ± 0.033 | 0.316 ± 0.010 | -             | 3.379 ± 0.056 | -             | 1.067 ± 0.016  | 0.821 ± 0.029 | 1.005 ± 0.022 | 1.613 ± 0.031 | 0.322 ± 0.007 | 0.567 ± 0.002 | 0.213 ± 0.004 |
| Ferulic acid ( <b>7</b> )         | 0.881 ± 0.022  | -             | 0.127 ± 0.004 | 0.138 ± 0.002 | -             | -             | 0.399 ± 0.014  | 0.222 ± 0.007 | 0.250 ± 0.012 | 0.220 ± 0.012 | 0.112 ± 0.006 | 0.146 ± 0.005 | 0.057 ± 0.003 |
| Benzoic acid ( <b>8</b> )         | -              | -             | -             | -             | 0.044 ± 0.002 | -             | -              | -             | -             | -             | -             | -             | -             |
| Senkyunolide I ( <b>9</b> )       | -              | 1.320 ± 0.016 | 0.852 ± 0.012 | 0.998 ± 0.024 | 0.900 ± 0.013 | 0.585 ± 0.007 | 0.922 ± 0.022  | 1.059 ± 0.020 | 0.529 ± 0.021 | 0.871 ± 0.014 | 0.468 ± 0.009 | 0.642 ± 0.008 | 0.287 ± 0.006 |
| Xanthotoxol ( <b>10</b> )         | -              | 0.039 ± 0.001 | -             | -             | 0.030 ± 0.001 | 0.025 ± 0.001 | 0.040 ± 0.000  | -             | -             | 0.025 ± 0.000 | 0.028 ± 0.001 | 0.026 ± 0.001 | -             |
| Senkyunolide H ( <b>11</b> )      | -              | 0.191 ± 0.004 | 0.115 ± 0.002 | 0.146 ± 0.004 | 0.127 ± 0.003 | 0.088 ± 0.002 | 0.128 ± 0.002  | 0.147 ± 0.006 | 0.086 ± 0.002 | 0.138 ± 0.002 | 0.076 ± 0.002 | 0.092 ± 0.002 | 0.045 ± 0.001 |
| Marmesin ( <b>12</b> )            | 1.640 ± 0.036  | -             | -             | -             | -             | 0.219 ± 0.002 | -              | -             | -             | -             | -             | -             | -             |
| Decursinol ( <b>15</b> )          | 1.760 ± 0.008  | -             | -             | 0.037 ± 0.000 | -             | 0.334 ± 0.002 | -              | -             | -             | -             | -             | 0.045 ± 0.002 | -             |
| Psoralen ( <b>18</b> )            | 0.231 ± 0.005  | 0.358 ± 0.005 | 0.086 ± 0.001 | 0.801 ± 0.020 | 0.910 ± 0.013 | 0.223 ± 0.002 | 0.696 ± 0.009  | 0.234 ± 0.004 | 0.091 ± 0.001 | 0.285 ± 0.004 | 0.153 ± 0.003 | 0.268 ± 0.003 | 0.053 ± 0.001 |
| Xanthotoxin ( <b>22</b> )         | 2.292 ± 0.049  | 2.267 ± 0.029 | 0.467 ± 0.006 | 3.473 ± 0.085 | 4.683 ± 0.071 | 1.004 ± 0.011 | 5.612 ± 0.074  | 1.295 ± 0.025 | 1.066 ± 0.019 | 3.640 ± 0.054 | 1.037 ± 0.021 | 1.549 ± 0.017 | 0.416 ± 0.009 |
| Bergapten ( <b>25</b> )           | 0.412 ± 0.009  | 0.522 ± 0.004 | 0.141 ± 0.006 | 0.657 ± 0.008 | 0.619 ± 0.011 | 0.186 ± 0.005 | 0.885 ± 0.011  | 0.444 ± 0.002 | 0.199 ± 0.002 | 0.480 ± 0.005 | 0.214 ± 0.005 | 0.388 ± 0.006 | 0.115 ± 0.004 |
| Coniferyl ferulate ( <b>31</b> )  | 3.663 ± 0.099  | -             | -             | -             | -             | 0.564 ± 0.016 | 0.298 ± 0.007  | -             | -             | -             | -             | 0.382 ± 0.006 | 0.189 ± 0.005 |
| Senkyunolide A ( <b>32</b> )      | -              | 0.343 ± 0.020 | 0.227 ± 0.006 | 0.305 ± 0.013 | 0.294 ± 0.004 | -             | 1.554 ± 0.016  | -             | -             | 0.504 ± 0.006 | 0.246 ± 0.006 | 0.378 ± 0.004 | 0.225 ± 0.005 |
| 3-n-Butyl-phthalide ( <b>33</b> ) | -              | 0.419 ± 0.008 | 0.171 ± 0.003 | 0.295 ± 0.008 | 0.363 ± 0.006 | 0.163 ± 0.002 | 0.709 ± 0.010  | 0.165 ± 0.004 | 0.083 ± 0.001 | 0.408 ± 0.007 | 0.163 ± 0.005 | 0.236 ± 0.004 | -             |
| Imperatorin ( <b>34</b> )         | -              | -             | -             | -             | -             | -             | 0.031 ± 0.000  | 0.011 ± 0.001 | -             | 0.017 ± 0.001 | 0.018 ± 0.001 | -             | -             |

|                             |                    |                  |                  |                  |                  |                   |                  |                  |                  |                  |                  |                   |                  |
|-----------------------------|--------------------|------------------|------------------|------------------|------------------|-------------------|------------------|------------------|------------------|------------------|------------------|-------------------|------------------|
| Ligustilide (35)            | -                  | 3.709 ±<br>0.045 | 2.320 ±<br>0.029 | 3.693 ±<br>0.090 | 3.302 ±<br>0.053 | 2.701 ±<br>0.029  | 5.030 ±<br>0.063 | 2.385 ±<br>0.047 | 5.735 ±<br>0.101 | 4.474 ±<br>0.068 | 4.407 ±<br>0.094 | 10.137 ±<br>0.121 | 6.647 ±<br>0.148 |
| Decursin (38)               | 132.507 ±<br>1.693 | 0.310 ±<br>0.004 | -                | -                | -                | 19.587 ±<br>0.236 | -                | -                | -                | -                | -                | -                 | -                |
| Decursinol<br>angelate (39) | 127.857 ±<br>2.712 | 0.214 ±<br>0.003 | -                | -                | -                | 22.420 ±<br>0.271 | -                | -                | -                | -                | -                | -                 | -                |
| Isoimperatorin<br>(40)      | -                  | 0.185 ±<br>0.003 | 0.188 ±<br>0.002 | 0.152 ±<br>0.004 | -                | -                 | 0.177 ±<br>0.002 | 0.217 ±<br>0.004 | 0.111 ±<br>0.002 | 0.143 ±<br>0.002 | 0.073 ±<br>0.001 | 0.232 ±<br>0.002  | --               |
| Falcarindiol<br>(43)        | -                  | 1.543 ±<br>0.012 | 0.632 ±<br>0.032 | 0.790 ±<br>0.034 | 0.699 ±<br>0.022 | -                 | 1.998 ±<br>0.034 | 1.048 ±<br>0.027 | 2.231 ±<br>0.034 | 2.623 ±<br>0.053 | 2.411 ±<br>0.050 | 1.910 ±<br>0.021  | 1.087 ±<br>0.031 |
| Levistilide A<br>(45)       | -                  | 0.419 ±<br>0.009 | 0.270 ±<br>0.006 | 0.290 ±<br>0.010 | 0.292 ±<br>0.006 | 0.148 ±<br>0.007  | 0.273 ±<br>0.015 | 0.384 ±<br>0.012 | 0.296 ±<br>0.008 | 0.281 ±<br>0.011 | 0.299 ±<br>0.010 | 0.331 ±<br>0.007  | 0.084 ±<br>0.003 |

AAC, *A.acutiloba*. The amounts of the marker compounds are expressed as 'Mean ± standard deviation'.

**Table S7.** Mean amounts of the marker compounds in the methanol extracts of *A. biserrata* samples (mg/g)

| Compound                               | ABI-01           | ABI -02          | ABI -03           | ABI-04            | ABI-05            | ABI-06            | ABI-07            | ABI-08            | ABI-09            | ABI-10            |
|--|------------------|------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| Chlorogenic acid ( <b>1</b> )          | 1.763 ±<br>0.110 | 2.110 ±<br>0.058 | 1.800 ±<br>0.031  | 4.049 ±<br>0.121  | 0.703 ±<br>0.033  | 4.725 ±<br>0.135  | 2.284 ±<br>0.023  | 7.309 ±<br>0.202  | 10.277 ±<br>0.071 | 4.353 ±<br>0.144  |
| Caffeic acid ( <b>2</b> )              | 0.134 ±<br>0.009 | 0.056 ±<br>0.003 | 0.356 ±<br>0.016  | 0.162 ±<br>0.006  | 0.692 ±<br>0.029  | 0.260 ±<br>0.012  | 0.063 ±<br>0.004  | 0.214 ±<br>0.010  | 0.225 ±<br>0.012  | 0.190 ±<br>0.011  |
| Umbelliferone ( <b>6</b> )             | -                | -                | 2.654 ±<br>0.068  | 1.896 ±<br>0.061  | 12.763 ±<br>0.089 | -                 | 0.609 ±<br>0.021  | -                 | 0.452 ±<br>0.009  | -                 |
| Ferulic acid ( <b>7</b> )              | 1.312 ±<br>0.047 | -                | -                 | -                 | -                 | 1.022 ±<br>0.028  | -                 | 0.202 ±<br>0.001  | 0.233 ±<br>0.002  | 0.080 ±<br>0.003  |
| Senkyunolide I ( <b>9</b> )            | 4.440 ±<br>0.143 | 0.813 ±<br>0.015 | -                 | -                 | -                 | 1.252 ±<br>0.027  | -                 | -                 | -                 | -                 |
| Senkyunolide H ( <b>11</b> )           | 0.798 ±<br>0.025 | 0.155 ±<br>0.003 | -                 | -                 | -                 | 0.238 ±<br>0.008  | 0.108 ±<br>0.002  | -                 | -                 | -                 |
| Marmesin ( <b>12</b> )                 | -                | 0.147 ±<br>0.003 | 0.281 ±<br>0.003  | -                 | 0.219 ±<br>0.004  | 0.437 ±<br>0.011  | -                 | -                 | -                 | -                 |
| Oxypeucedanin<br>hydrate ( <b>14</b> ) | -                | 0.107 ±<br>0.002 | -                 | -                 | -                 | -                 | -                 | 0.112 ±<br>0.005  | -                 | -                 |
| Bergaptol ( <b>16</b> )                | -                | -                | -                 | -                 | -                 | -                 | 1.951 ±<br>0.012  | -                 | -                 | -                 |
| Byakangelicin ( <b>17</b> )            | -                | 0.049 ±<br>0.001 | -                 | -                 | 0.144 ±<br>0.001  | -                 | -                 | 0.050 ±<br>0.000  | -                 | -                 |
| Psoralen ( <b>18</b> )                 | -                | 0.031 ±<br>0.001 | 0.393 ±<br>0.003  | 0.302 ±<br>0.006  | 0.041 ±<br>0.001  | 0.812 ±<br>0.014  | 0.860 ±<br>0.009  | -                 | -                 | -                 |
| Angelol B ( <b>19</b> )                | -                | -                | 5.938 ±<br>0.048  | 7.756 ±<br>0.150  | -                 | 1.279 ±<br>0.026  | 0.120 ±<br>0.001  | 0.096 ±<br>0.001  | 0.209 ±<br>0.003  | -                 |
| Angelol H ( <b>20</b> )                | -                | -                | 2.321 ±<br>0.053  | 2.764 ±<br>0.054  | -                 | 0.388 ±<br>0.010  | 4.341 ±<br>0.116  | 1.461 ±<br>0.015  | 5.533 ±<br>0.063  | 1.154 ±<br>0.014  |
| Angelicin ( <b>21</b> )                | -                | 0.109 ±<br>0.001 | -                 | -                 | 0.265 ±<br>0.002  | -                 | 1.527 ±<br>0.077  | 0.329 ±<br>0.006  | 1.755 ±<br>0.052  | 0.348 ±<br>0.013  |
| Xanthotoxin ( <b>22</b> )              | -                | 0.030 ±<br>0.000 | 0.401 ±<br>0.006  | 1.156 ±<br>0.020  | 0.064 ±<br>0.001  | 2.250 ±<br>0.044  | -                 | -                 | -                 | -                 |
| Angelol A ( <b>23</b> )                | -                | -                | 34.523 ±<br>0.393 | 37.441 ±<br>0.671 | -                 | 8.977 ±<br>0.180  | 0.527 ±<br>0.006  | 0.361 ±<br>0.003  | 0.733 ±<br>0.010  | 0.059 ±<br>0.002  |
| Angelol G ( <b>24</b> )                | -                | -                | 8.995 ±<br>0.078  | 12.505 ±<br>0.228 | -                 | 19.749 ±<br>0.408 | 20.928 ±<br>0.207 | 6.367 ±<br>0.027  | 16.795 ±<br>0.172 | 6.777 ±<br>0.070  |
| Bergapten ( <b>25</b> )                | -                | 0.103 ±<br>0.002 | 0.328 ±<br>0.004  | 0.649 ±<br>0.013  | 0.206 ±<br>0.002  | 0.811 ±<br>0.034  | 11.368 ±<br>0.146 | 18.844 ±<br>0.086 | 21.964 ±<br>0.239 | 12.405 ±<br>0.127 |

|  |                   |                   |                   |                   |                   |                  |                   |                   |                   |                   |
|--|-------------------|-------------------|-------------------|-------------------|-------------------|------------------|-------------------|-------------------|-------------------|-------------------|
| Ostenol ( <b>26</b> )                  | -                 | 0.448 ±<br>0.009  | 0.128 ±<br>0.001  | 0.521 ±<br>0.010  | 2.138 ±<br>0.016  | 0.229 ±<br>0.004 | 0.710 ±<br>0.006  | 0.521 ±<br>0.003  | 0.362 ±<br>0.004  | 0.055 ±<br>0.002  |
| Bisabolangelone ( <b>27</b> )          | -                 | -                 | 1.280 ±<br>0.014  | 2.419 ±<br>0.037  | -                 | 3.444 ±<br>0.068 | 0.247 ±<br>0.004  | 0.218 ±<br>0.001  | 0.439 ±<br>0.004  | 0.298 ±<br>0.003  |
| Byakangelicol ( <b>28</b> )            | -                 | -                 | -                 | -                 | -                 | -                | 6.933 ±<br>0.058  | 1.847 ±<br>0.016  | 0.873 ±<br>0.006  | 1.310 ±<br>0.014  |
| Columbianetin acetate<br>( <b>30</b> ) | -                 | -                 | 1.800 ±<br>0.022  | 8.089 ±<br>0.144  | -                 | 2.176 ±<br>0.045 | 0.574 ±<br>0.004  | -                 | -                 | -                 |
| Coniferyl ferulate ( <b>31</b> )       | 0.915 ±<br>0.032  | 2.409 ±<br>0.011  | -                 | -                 | -                 | 0.954 ±<br>0.020 | 4.054 ±<br>0.034  | 7.133 ±<br>0.032  | 7.494 ±<br>0.087  | 7.478 ±<br>0.073  |
| Imperatorin ( <b>34</b> )              | -                 | -                 | -                 | -                 | -                 | 0.068 ±<br>0.002 | -                 | 0.897 ±<br>0.022  | -                 | -                 |
| Ligustilide ( <b>35</b> )              | 14.490 ±<br>0.456 | 10.532 ±<br>0.182 | -                 | -                 | -                 | 9.090 ±<br>0.176 | 5.639 ±<br>0.058  | 0.023 ±<br>0.000  | 0.050 ±<br>0.001  | 0.030 ±<br>0.001  |
| Osthol ( <b>37</b> )                   | -                 | -                 | 13.162 ±<br>0.168 | 47.805 ±<br>0.840 | -                 | 9.791 ±<br>0.197 | -                 | -                 | -                 | -                 |
| Decursin ( <b>38</b> )                 | -                 | -                 | -                 | -                 | -                 | -                | 3.047 ±<br>0.036  | -                 | -                 | -                 |
| Decursinol angelate<br>( <b>39</b> )   | -                 | -                 | -                 | -                 | -                 | -                | 0.466 ±<br>0.008  | 26.883 ±<br>0.118 | 22.876 ±<br>0.241 | 21.571 ±<br>0.205 |
| Isoimperatorin ( <b>40</b> )           | -                 | -                 | 0.656 ±<br>0.008  | 0.765 ±<br>0.014  | -                 | 0.369 ±<br>0.007 | -                 | -                 | -                 | -                 |
| Suberosin ( <b>41</b> )                | -                 | 3.014 ±<br>0.065  | -                 | -                 | -                 | -                | -                 | -                 | -                 | -                 |
| Columbianadin ( <b>42</b> )            | -                 | -                 | 6.457 ±<br>0.077  | 15.515 ±<br>0.276 | 10.574 ±<br>0.086 | 7.637 ±<br>0.155 | 2.106 ±<br>0.031  | 1.342 ±<br>0.008  | 0.854 ±<br>0.001  | 0.547 ±<br>0.006  |
| Falcarindiol ( <b>43</b> )             | 11.317 ±<br>0.388 | 2.955 ±<br>0.174  | -                 | -                 | -                 | 7.475 ±<br>0.080 | -                 | -                 | -                 | -                 |
| Praeruptorin B ( <b>44</b> )           | -                 | 3.727 ±<br>0.071  | -                 | -                 | 5.690 ±<br>0.047  | -                | 16.830 ±<br>0.169 | 3.619 ±<br>0.017  | 16.020 ±<br>0.171 | 2.996 ±<br>0.029  |
| Levistilide A ( <b>45</b> )            | 4.038 ±<br>0.136  | 2.040 ±<br>0.035  | -                 | -                 | -                 | 1.434 ±<br>0.054 | 2.206 ±<br>0.011  | -                 | -                 | -                 |
| Praeruptorin C ( <b>46</b> )           | -                 | 0.694 ±<br>0.009  | -                 | -                 | -                 | -                | -                 | -                 | -                 | -                 |

ABI, *A. biserrata*. The amounts of the marker compounds are expressed as ‘Mean ± standard deviation’.

**Table S8.** Mean amounts of the marker compounds in the methanol extracts of *A. dahurica* samples (mg/g)

| Compound                               | ADA-01        | ADA-02        | ADA-03        | ADA-04        | ADA-05        | ADA-06         | ADA-07        | ADA-08         | ADA-09        | ADA-10         | ADA-11        | ADA-12         | ADA-13        | ADA-14        | ADA-15         |
|--|---------------|---------------|---------------|---------------|---------------|----------------|---------------|----------------|---------------|----------------|---------------|----------------|---------------|---------------|----------------|
| Chlorogenic acid ( <b>1</b> )          | 5.321 ± 0.191 | 0.824 ± 0.024 | 2.882 ± 0.094 | 3.780 ± 0.127 | 3.408 ± 0.035 | 3.501 ± 0.056  | 1.119 ± 0.019 | 4.975 ± 0.111  | 0.844 ± 0.012 | 3.580 ± 0.094  | 4.567 ± 0.138 | 12.251 ± 0.209 | 1.956 ± 0.060 | 2.620 ± 0.024 | 5.612 ± 0.142  |
| Caffeic acid ( <b>2</b> )              | 0.317 ± 0.008 | 0.093 ± 0.007 | 0.122 ± 0.002 | 0.175 ± 0.005 | 0.263 ± 0.005 | 0.763 ± 0.014  | 0.163 ± 0.004 | 0.174 ± 0.005  | 0.067 ± 0.002 | 0.115 ± 0.001  | 0.246 ± 0.005 | 0.196 ± 0.006  | 0.059 ± 0.002 | 0.156 ± 0.004 | 0.194 ± 0.007  |
| Prim-O-glucosyl-cimifugin ( <b>3</b> ) | -             | -             | -             | -             | -             | 7.348 ± 0.046  | -             | 4.871 ± 0.120  | -             | -              | -             | -              | -             | -             | -              |
| Ferulic acid ( <b>7</b> )              | 0.210 ± 0.004 | -             | 0.088 ± 0.003 | 0.333 ± 0.005 | 0.119 ± 0.003 | 0.486 ± 0.008  | 0.047 ± 0.002 | 0.298 ± 0.003  | 0.056 ± 0.003 | 0.292 ± 0.003  | 0.185 ± 0.008 | 0.382 ± 0.003  | 0.177 ± 0.004 | 0.194 ± 0.003 | 0.305 ± 0.003  |
| Xanthotoxol ( <b>10</b> )              | 0.069 ± 0.001 | 0.095 ± 0.001 | 0.099 ± 0.001 | 0.086 ± 0.001 | 1.206 ± 0.005 | 0.109 ± 0.001  | 1.196 ± 0.016 | 0.321 ± 0.003  | 0.310 ± 0.004 | 0.275 ± 0.007  | 0.135 ± 0.002 | 0.173 ± 0.002  | 0.190 ± 0.006 | 0.174 ± 0.002 | 0.345 ± 0.003  |
| Marmesin ( <b>12</b> )                 | -             | 0.037 ± 0.001 | 0.064 ± 0.004 | 0.069 ± 0.001 | 0.104 ± 0.001 | 0.151 ± 0.001  | -             | 0.091 ± 0.003  | 0.099 ± 0.002 | 0.213 ± 0.006  | 0.157 ± 0.000 | 0.061 ± 0.001  | 0.077 ± 0.000 | 0.091 ± 0.002 | 0.269 ± 0.004  |
| Oxypeucedanin hydrate ( <b>14</b> )    | 2.621 ± 0.047 | 3.734 ± 0.068 | 4.231 ± 0.053 | 4.925 ± 0.047 | 8.477 ± 0.072 | 8.519 ± 0.082  | 5.930 ± 0.059 | 9.788 ± 0.200  | 6.628 ± 0.090 | 14.484 ± 0.376 | 7.710 ± 0.086 | 7.406 ± 0.077  | 8.077 ± 0.195 | 5.843 ± 0.054 | 10.514 ± 0.079 |
| Byakangelicin ( <b>17</b> )            | 3.148 ± 0.013 | 2.767 ± 0.049 | 3.582 ± 0.046 | 7.228 ± 0.127 | 3.446 ± 0.033 | 10.603 ± 0.088 | 2.597 ± 0.026 | 12.003 ± 0.043 | 6.229 ± 0.098 | 21.371 ± 0.523 | 8.988 ± 0.099 | 6.986 ± 0.070  | 9.565 ± 0.107 | 5.946 ± 0.059 | 15.621 ± 0.179 |
| Psoralen ( <b>18</b> )                 | 0.223 ± 0.005 | 0.150 ± 0.003 | 0.354 ± 0.005 | 0.357 ± 0.006 | 0.075 ± 0.001 | 0.299 ± 0.005  | -             | 0.111 ± 0.002  | 0.406 ± 0.006 | 2.008 ± 0.049  | 0.489 ± 0.006 | 0.804 ± 0.008  | 0.108 ± 0.005 | 0.125 ± 0.001 | 0.649 ± 0.032  |
| Xanthotoxin ( <b>22</b> )              | 0.104 ± 0.003 | 0.296 ± 0.006 | 0.322 ± 0.005 | 0.305 ± 0.004 | 1.296 ± 0.010 | 0.215 ± 0.002  | 0.032 ± 0.000 | 0.334 ± 0.003  | 0.461 ± 0.007 | 3.715 ± 0.091  | 0.495 ± 0.006 | 0.717 ± 0.008  | 0.104 ± 0.002 | 0.100 ± 0.001 | 0.643 ± 0.045  |
| Angelol A ( <b>23</b> )                | 0.106 ± 0.003 | 0.171 ± 0.005 | 0.213 ± 0.005 | 0.094 ± 0.002 | 0.286 ± 0.006 | 0.161 ± 0.002  | 0.257 ± 0.003 | 0.313 ± 0.006  | 0.178 ± 0.003 | 1.032 ± 0.024  | 0.166 ± 0.003 | 0.186 ± 0.003  | 0.151 ± 0.004 | 0.155 ± 0.003 | 0.429 ± 0.003  |
| Bergapten ( <b>25</b> )                | 0.109 ± 0.003 | 1.030 ± 0.021 | 1.417 ± 0.022 | 0.268 ± 0.003 | 1.949 ± 0.016 | 0.366 ± 0.003  | 0.802 ± 0.009 | 0.538 ± 0.008  | 1.283 ± 0.019 | 0.859 ± 0.017  | 0.318 ± 0.003 | 0.317 ± 0.003  | 0.346 ± 0.007 | 0.248 ± 0.002 | 0.409 ± 0.003  |

|                                 |                   |                   |                   |                   |                   |                   |                   |                   |                   |                   |                  |                  |                   |                  |                   |
|---------------------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|------------------|------------------|-------------------|------------------|-------------------|
| Ostenol ( <b>26</b> )           | 0.056 ±<br>0.001  | 0.157 ±<br>0.005  | 0.131 ±<br>0.002  | -                 | 0.620 ±<br>0.006  | -                 | 0.708 ±<br>0.002  | -                 | -                 | 0.141 ±<br>0.001  | -                | -                | -                 | -                |                   |
| Byakangelicol<br>( <b>28</b> )  | 6.054 ±<br>0.184  | 2.568 ±<br>0.069  | 6.890 ±<br>0.136  | 18.701<br>± 0.385 | 0.256 ±<br>0.002  | 14.560<br>± 0.261 | -                 | 11.341<br>± 0.059 | 0.956 ±<br>0.025  | 27.402<br>± 0.846 | 5.383 ±<br>0.067 | 5.044<br>± 0.109 | 12.510<br>± 0.324 | 3.830<br>± 0.058 | 13.913<br>± 0.172 |
| Oxypeucedanin<br>( <b>29</b> )  | 10.410<br>± 0.298 | 8.204 ±<br>0.206  | 17.018<br>± 0.317 | 21.605<br>± 0.408 | 1.241 ±<br>0.015  | 19.268<br>± 0.309 | 1.457 ±<br>0.023  | 23.185<br>± 0.128 | 4.192 ±<br>0.077  | 26.353<br>± 0.773 | 5.389 ±<br>0.062 | 7.629<br>± 0.106 | 17.734<br>± 0.431 | 6.153<br>± 0.085 | 11.651<br>± 0.079 |
| Imperatorin<br>( <b>34</b> )    | 5.570 ±<br>0.137  | 11.129<br>± 0.236 | 7.171 ±<br>0.112  | 5.667 ±<br>0.083  | 21.347<br>± 0.186 | 15.830<br>± 0.179 | 29.245<br>± 0.330 | 11.613<br>± 0.093 | 11.269<br>± 0.178 | 8.968 ±<br>0.225  | 5.891 ±<br>0.069 | 4.100<br>± 0.045 | 10.037<br>± 0.222 | 8.647<br>± 0.098 | 19.399<br>± 0.187 |
| Phellopterin<br>( <b>36</b> )   | 2.643 ±<br>0.064  | 7.605 ±<br>0.160  | 6.280 ±<br>0.099  | 4.239 ±<br>0.061  | 20.727<br>± 0.093 | 8.172 ±<br>0.092  | 31.988<br>± 0.355 | 12.909<br>± 0.111 | 7.879 ±<br>0.125  | 7.617 ±<br>0.191  | 3.849 ±<br>0.043 | 3.893<br>± 0.042 | 9.108 ±<br>0.232  | 5.466<br>± 0.055 | 11.286<br>± 0.111 |
| Decursin ( <b>38</b> )          | -                 | 0.119 ±<br>0.002  | -                 | -                 | -                 | -                 | -                 | -                 | -                 | -                 | -                | -                | -                 | -                |                   |
| Isoimperatorin<br>( <b>40</b> ) | 5.194 ±<br>0.124  | 4.596 ±<br>0.093  | 4.839 ±<br>0.072  | 9.264 ±<br>0.132  | 14.940<br>± 0.155 | 12.637<br>± 0.129 | 17.641<br>± 0.206 | 16.698<br>± 0.145 | 5.017 ±<br>0.072  | 15.057<br>± 0.372 | 6.370 ±<br>0.081 | 6.312<br>± 0.062 | 11.631<br>± 0.251 | 6.752<br>± 0.071 | 13.421<br>± 0.120 |
| Suberosin ( <b>41</b> )         | -                 | 0.521 ±<br>0.012  | 0.167 ±<br>0.006  | -                 | 0.542 ±<br>0.002  | -                 | 0.140 ±<br>0.003  | 0.268 ±<br>0.006  | 0.365 ±<br>0.009  | -                 | 0.189 ±<br>0.003 | -                | -                 | -                |                   |
| Falcarindiol<br>( <b>43</b> )   | 1.023 ±<br>0.016  | 3.379 ±<br>0.089  | 5.151 ±<br>0.092  | 1.747 ±<br>0.006  | 15.614<br>± 0.154 | 1.196 ±<br>0.022  | 9.696 ±<br>0.104  | 2.969 ±<br>0.046  | 5.031 ±<br>0.180  | -                 | 0.850 ±<br>0.037 | 1.391<br>± 0.038 | 2.439 ±<br>0.074  | 1.811<br>± 0.044 | 4.456 ±<br>0.112  |

ADA, *A.dahurica*. The amounts of the marker compounds are expressed as ‘Mean ± standard deviation’.

**Table S9.** Mean amounts of the marker compounds in the methanol extracts of *A. decursiva* samples (mg/g)

| Compound                          | ADE-01        | ADE-02         | ADE-03         | ADE-04         | ADE-05         | ADE-06         | ADE-07        | ADE-08         | ADE-09         | ADE-10         | ADE-11         | ADE-12         | ADE-13         |
|-----------------------------------|---------------|----------------|----------------|----------------|----------------|----------------|---------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Chlorogenic acid ( <b>1</b> )     | 0.518 ± 0.012 | 0.192 ± 0.005  | 0.274 ± 0.008  | 0.266 ± 0.008  | 0.405 ± 0.024  | 1.280 ± 0.030  | 0.165 ± 0.008 | 0.723 ± 0.040  | 6.826 ± 0.233  | 6.944 ± 0.052  | 5.476 ± 0.142  | 6.003 ± 0.161  | 4.052 ± 0.178  |
| Nodakenin ( <b>5</b> )            | 3.483 ± 0.265 | -              | -              | -              | -              | -              | -             | -              | 67.853 ± 0.461 | 56.985 ± 0.698 | 89.051 ± 0.905 | 63.972 ± 0.410 | 74.029 ± 2.153 |
| Umbelliferone (6)                 | 5.016 ± 0.106 | 3.971 ± 0.033  | 3.356 ± 0.064  | 4.677 ± 0.046  | 5.164 ± 0.041  | 4.244 ± 0.088  | 4.632 ± 0.066 | 4.354 ± 0.090  | -              | -              | -              | -              | -              |
| Marmesin ( <b>12</b> )            | 0.930 ± 0.026 | 0.062 ± 0.001  | 0.064 ± 0.001  | 0.031 ± 0.000  | 0.045 ± 0.001  | 0.171 ± 0.004  | 0.063 ± 0.001 | 0.152 ± 0.006  | 0.557 ± 0.004  | 0.624 ± 0.007  | 0.539 ± 0.006  | 0.489 ± 0.001  | 0.369 ± 0.011  |
| Decursinol ( <b>15</b> )          | 0.083 ± 0.003 | 0.041 ± 0.000  | 0.030 ± 0.000  | -              | -              | 0.050 ± 0.001  | 0.042 ± 0.001 | 0.038 ± 0.001  | 0.092 ± 0.003  | 0.078 ± 0.005  | 0.111 ± 0.003  | 0.046 ± 0.001  | 0.058 ± 0.002  |
| Psoralen ( <b>18</b> )            | 0.180 ± 0.000 | 0.059 ± 0.005  | 0.081 ± 0.003  | 0.052 ± 0.001  | 0.051 ± 0.001  | 0.512 ± 0.014  | 0.039 ± 0.004 | 0.189 ± 0.004  | -              | -              | -              | -              | -              |
| Xanthotoxin (22)                  | 0.643 ± 0.016 | 0.245 ± 0.002  | 0.192 ± 0.002  | 0.115 ± 0.001  | 0.209 ± 0.001  | 0.636 ± 0.024  | 0.308 ± 0.005 | 0.674 ± 0.014  | 0.022 ± 0.000  | -              | -              | -              | -              |
| Bergapten ( <b>25</b> )           | 0.240 ± 0.008 | 0.390 ± 0.003  | 0.351 ± 0.004  | 0.306 ± 0.003  | 0.313 ± 0.003  | 0.584 ± 0.011  | 0.361 ± 0.006 | 0.597 ± 0.012  | 0.030 ± 0.000  | 0.035 ± 0.000  | -              | -              | -              |
| Ostenol ( <b>26</b> )             | 0.182 ± 0.020 | 0.109 ± 0.001  | 0.083 ± 0.001  | 0.104 ± 0.004  | 0.094 ± 0.003  | 0.272 ± 0.009  | 0.104 ± 0.001 | 0.116 ± 0.003  | -              | -              | -              | -              | -              |
| Bisabolangelo ne (27)             | 1.288 ± 0.018 | 0.867 ± 0.003  | 0.709 ± 0.007  | 0.023 ± 0.002  | -              | -              | 0.357 ± 0.006 | -              | -              | -              | -              | -              | -              |
| Coniferyl ferulate ( <b>31</b> )  | 2.471 ± 0.121 | -              | -              | -              | -              | -              | -             | -              | 5.085 ± 0.125  | 2.873 ± 0.066  | 4.340 ± 0.045  | 3.703 ± 0.047  | 4.087 ± 0.057  |
| Decursin ( <b>38</b> )            | 0.842 ± 0.008 | 0.317 ± 0.002  | 0.280 ± 0.005  | 0.198 ± 0.003  | 0.208 ± 0.004  | 0.314 ± 0.007  | 0.316 ± 0.012 | 0.309 ± 0.007  | 3.586 ± 0.026  | 0.926 ± 0.012  | 2.991 ± 0.035  | 0.609 ± 0.002  | 2.229 ± 0.065  |
| Decursinol angelate ( <b>39</b> ) | -             | -              | -              | -              | -              | -              | -             | -              | 6.797 ± 0.058  | 4.250 ± 0.047  | 7.481 ± 0.085  | 3.514 ± 0.014  | 5.539 ± 0.167  |
| Columbianadin ( <b>42</b> )       | -             | -              | -              | -              | -              | -              | -             | -              | 2.708 ± 0.074  | 2.118 ± 0.102  | 4.333 ± 0.064  | 0.966 ± 0.004  | 1.708 ± 0.092  |
| Falcarindiol ( <b>43</b> )        | 5.886 ± 0.204 | 11.645 ± 0.042 | 13.255 ± 0.196 | 14.360 ± 0.157 | 14.219 ± 0.108 | 10.850 ± 0.206 | 9.389 ± 0.143 | 12.485 ± 0.259 | -              | -              | 1.189 ± 0.021  | -              | -              |

ADE, *A. decursiva*. The amounts of the marker compounds are expressed as ‘Mean ± standard deviation’.

**Table S10.** Mean amounts of the marker compounds in the methanol extracts of *A. gigas* samples (mg/g)

| Compound                          | AGI-01            | AGI-02             | AGI-03             | AGI-04             | AGI-05            | AGI-06             | AGI-07             | AGI-08             | AGI-09            | AGI-10             | AGI-11            |
|-----------------------------------|-------------------|--------------------|--------------------|--------------------|-------------------|--------------------|--------------------|--------------------|-------------------|--------------------|-------------------|
| Chlorogenic acid ( <b>1</b> )     | 10.024 ±<br>0.307 | 9.205 ±<br>0.202   | 9.491 ±<br>0.349   | 12.128 ±<br>0.287  | 10.910 ±<br>0.031 | 5.122 ±<br>0.098   | 11.007 ±<br>0.203  | 10.269 ±<br>0.147  | 12.684 ±<br>0.089 | 13.471 ±<br>0.431  | 9.456 ±<br>0.247  |
| Caffeic acid ( <b>2</b> )         | 0.144 ±<br>0.008  | 0.279 ±<br>0.009   | 0.565 ±<br>0.024   | 0.103 ±<br>0.002   | 0.101 ±<br>0.003  | 0.077 ±<br>0.003   | 0.226 ±<br>0.003   | 0.296 ±<br>0.003   | 0.376 ±<br>0.009  | 0.196 ±<br>0.005   | 0.043 ±<br>0.001  |
| Nodakenin ( <b>5</b> )            | 15.025 ±<br>0.293 | 26.372 ±<br>0.345  | 23.284 ±<br>0.534  | 15.187 ±<br>0.231  | 17.472 ±<br>0.113 | 18.660 ±<br>0.323  | 19.279 ±<br>0.266  | 30.228 ±<br>0.379  | 21.818 ±<br>0.211 | 15.088 ±<br>±0.235 | 9.805 ±<br>0.089  |
| Marmesin ( <b>12</b> )            | 0.746 ±<br>0.019  | 1.504 ±<br>0.018   | 1.449 ±<br>0.036   | 0.737 ±<br>0.031   | 0.726 ±<br>0.006  | 0.398 ±<br>0.017   | 0.874 ±<br>0.013   | 2.211 ±<br>0.022   | 1.144 ±<br>0.009  | 0.566 ±<br>0.013   | 0.416 ±<br>0.007  |
| Decursinol ( <b>15</b> )          | 2.061 ±<br>0.022  | 1.536 ±<br>0.020   | 1.776 ±<br>0.018   | 2.706 ±<br>0.019   | 1.574 ±<br>0.030  | 3.651 ±<br>0.048   | 1.993 ±<br>0.025   | 2.870 ±<br>0.027   | 0.891 ±<br>0.004  | 0.924 ±<br>0.003   | 0.538 ±<br>0.008  |
| Psoralen ( <b>18</b> )            | 0.047 ±<br>0.001  | 0.065 ±<br>0.001   | 0.250 ±<br>0.006   | 0.332 ±<br>0.007   | 0.150 ±<br>0.001  | 0.041 ±<br>0.001   | 0.278 ±<br>0.003   | 2.623 ±<br>0.030   | 0.097 ±<br>0.001  | 0.032 ±<br>0.001   | 0.122 ±<br>0.002  |
| Xanthotoxin ( <b>22</b> )         | 0.048 ±<br>0.002  | 0.186 ±<br>0.003   | 0.795 ±<br>0.018   | 0.477 ±<br>0.010   | 0.602 ±<br>0.005  | 0.012 ±<br>0.000   | 0.804 ±<br>0.012   | 7.707 ±<br>0.087   | 0.555 ±<br>0.007  | 0.058 ±<br>0.001   | 0.437 ±<br>0.007  |
| Bergapten ( <b>25</b> )           | 0.100 ±<br>0.002  | 0.154 ±<br>0.002   | 0.336 ±<br>0.008   | 0.185 ±<br>0.003   | 0.147 ±<br>0.001  | 0.067 ±<br>0.001   | 0.213 ±<br>0.003   | 0.688 ±<br>0.006   | 0.279 ±<br>0.004  | 0.152 ±<br>0.005   | 0.189 ±<br>0.003  |
| Coniferyl ferulate ( <b>31</b> )  | 0.330 ±<br>0.014  | 1.618 ±<br>0.060   | 2.291 ±<br>0.078   | 0.445 ±<br>0.016   | 0.434 ±<br>0.009  | 0.698 ±<br>0.010   | 0.832 ±<br>0.023   | 2.371 ±<br>0.020   | 3.673 ±<br>0.047  | 0.847 ±<br>0.025   | 3.300 ±<br>0.105  |
| Imperatorin ( <b>34</b> )         | 0.044 ±<br>0.001  | 0.330 ±<br>0.004   | 0.064 ±<br>0.002   | -                  | 0.032 ±<br>0.001  | 0.069 ±<br>0.002   | 0.040 ±<br>0.000   | 0.258 ±<br>0.004   | 0.025 ±<br>0.000  | 0.044 ±<br>0.001   | 0.019 ±<br>0.001  |
| Decursin ( <b>38</b> )            | 88.211 ±<br>1.916 | 125.015 ±<br>1.189 | 120.429 ±<br>2.111 | 97.499 ±<br>1.953  | 88.387 ±<br>0.686 | 116.643 ±<br>1.575 | 107.347 ±<br>1.255 | 132.719 ±<br>0.946 | 92.042 ±<br>1.029 | 84.618 ±<br>1.739  | 93.120 ±<br>1.460 |
| Decursinol angelate ( <b>39</b> ) | 91.762 ±<br>2.151 | 108.000 ±<br>1.333 | 102.472 ±<br>2.426 | 107.230 ±<br>2.295 | 52.677 ±<br>0.462 | 192.851 ±<br>2.336 | 103.926 ±<br>1.431 | 102.543 ±<br>1.246 | 88.822 ±<br>1.092 | 70.031 ±<br>1.531  | 78.624 ±<br>1.327 |
| Suberosin ( <b>41</b> )           | -                 | 0.195 ±<br>0.013   | -                  | -                  | -                 | -                  | -                  | -                  | -                 | -                  | 0.247 ±<br>0.004  |

AGI, *Angelica gigas*. The amounts of the marker compounds are expressed as ‘Mean ± standard deviation’.

**Table S11.** Mean amounts of the marker compounds in the methanol extracts of *A. polymorpha* samples (mg/g)

| Compound                            | APO-01         | APO-02         | APO-03         | APO-04        | APO-05         | APO-06         |
|-------------------------------------|----------------|----------------|----------------|---------------|----------------|----------------|
| Chlorogenic acid ( <b>1</b> )       | 1.212 ± 0.041  | 2.970 ± 0.105  | 5.994 ± 0.291  | 3.316 ± 0.063 | 4.810 ± 0.153  | 0.462 ± 0.007  |
| Ferulic acid ( <b>7</b> )           | 1.296 ± 0.024  | 0.994 ± 0.014  | 1.204 ± 0.009  | 0.562 ± 0.032 | 2.108 ± 0.043  | 0.321 ± 0.012  |
| Marmesin ( <b>12</b> )              | 0.177 ± 0.006  | 0.036 ± 0.001  | 0.223 ± 0.003  | 0.035 ± 0.002 | 0.151 ± 0.001  | 0.189 ± 0.001  |
| Oxypeucedanin hydrate ( <b>14</b> ) | 1.338 ± 0.015  | 0.437 ± 0.008  | 2.518 ± 0.066  | 0.335 ± 0.003 | 3.118 ± 0.058  | 1.644 ± 0.008  |
| Byakangelicin ( <b>17</b> )         | 0.787 ± 0.020  | 0.164 ± 0.005  | 1.397 ± 0.025  | 0.141 ± 0.002 | 1.957 ± 0.053  | 0.459 ± 0.012  |
| Bergapten ( <b>25</b> )             | 0.614 ± 0.014  | 0.151 ± 0.004  | 1.769 ± 0.044  | 0.071 ± 0.000 | 5.311 ± 0.132  | 0.252 ± 0.002  |
| Byakangelicol ( <b>28</b> )         | 2.816 ± 0.059  | 0.751 ± 0.012  | 5.657 ± 0.146  | 0.746 ± 0.005 | 11.002 ± 0.219 | 1.932 ± 0.013  |
| Oxypeucedanin ( <b>29</b> )         | 9.966 ± 0.213  | 4.326 ± 0.066  | 24.752 ± 0.613 | 3.556 ± 0.019 | 40.843 ± 0.824 | 12.899 ± 0.085 |
| Coniferyl ferulate ( <b>31</b> )    | 8.533 ± 0.382  | 3.194 ± 0.118  | 4.135 ± 0.233  | 3.266 ± 0.151 | 6.177 ± 0.463  | 2.635 ± 0.109  |
| Imperatorin ( <b>34</b> )           | 0.058 ± 0.003  | 0.073 ± 0.001  | 1.401 ± 0.032  | 0.055 ± 0.000 | 0.240 ± 0.007  | 0.892 ± 0.005  |
| Phellopterin ( <b>36</b> )          | 0.541 ± 0.012  | 0.189 ± 0.002  | 1.336 ± 0.034  | 0.297 ± 0.002 | 1.340 ± 0.033  | 0.821 ± 0.007  |
| Isoimperatorin ( <b>40</b> )        | 2.997 ± 0.074  | 0.977 ± 0.012  | 7.907 ± 0.211  | 1.171 ± 0.005 | 5.341 ± 0.108  | 4.991 ± 0.026  |
| Suberosin ( <b>41</b> )             | 0.400 ± 0.008  | 0.052 ± 0.002  | 0.356 ± 0.011  | 0.037 ± 0.000 | 0.249 ± 0.004  | 0.253 ± 0.002  |
| Falcarindiol ( <b>43</b> )          | 30.960 ± 0.765 | 16.437 ± 0.220 | 29.615 ± 0.738 | 6.836 ± 0.042 | 54.795 ± 1.012 | 16.726 ± 0.072 |

APO, *A. polymorpha*. The amounts of the marker compounds are expressed as ‘Mean ± standard deviation’.

**Table S12.** Mean amounts of the marker compounds in the methanol extracts of *A. reflexa* samples (mg/g)

| Compound                      | ARE-01            | ARE-02            | ARE-03           | ARE-04           | ARE-05            | ARE-06           | ARE-07           | ARE-08            | ARE-09           | ARE-10           | ARE-11           | ARE-12            |
|-------------------------------|-------------------|-------------------|------------------|------------------|-------------------|------------------|------------------|-------------------|------------------|------------------|------------------|-------------------|
| Chlorogenic acid<br>(1)       | 7.694 ±<br>0.369  | 8.596 ±<br>0.176  | 9.285 ±<br>0.119 | 7.997 ±<br>0.084 | 14.301 ±<br>0.427 | 4.589 ±<br>0.050 | 3.778 ±<br>0.032 | 8.762 ±<br>0.188  | 9.109 ±<br>0.143 | 8.507 ±<br>0.074 | 9.919 ±<br>0.180 | 5.664 ±<br>0.113  |
| Caffeic acid (2)              | 0.381 ±<br>0.018  | 0.390 ±<br>0.013  | 0.358 ±<br>0.016 | 0.188 ±<br>0.006 | 0.188 ±<br>0.005  | 0.119 ±<br>0.002 | 0.297 ±<br>0.008 | 0.412 ±<br>0.009  | 0.357 ±<br>0.007 | 0.225 ±<br>0.001 | 0.190 ±<br>0.004 | 0.269 ±<br>0.004  |
| Prim-O-glucosyl-cimifugin (3) | 2.420 ±<br>0.092  | 2.880 ±<br>0.075  | -                | -                | 4.357 ±<br>0.059  | -                | -                | 2.530 ±<br>0.064  | 2.788 ±<br>0.061 | -                | -                | 4.952 ±<br>0.018  |
| Cimifugin (4)                 | 2.321 ±<br>0.093  | 1.379 ±<br>0.024  | -                | -                | 0.915 ±<br>0.031  | -                | -                | 2.258 ±<br>0.048  | 1.181 ±<br>0.015 | -                | -                | 2.111 ±<br>0.014  |
| Ferulic acid (7)              | 0.678 ±<br>0.023  | 1.146 ±<br>0.011  | 2.593 ±<br>0.014 | 3.097 ±<br>0.058 | 0.968 ±<br>0.012  | 5.947 ±<br>0.034 | 2.390 ±<br>0.012 | 0.692 ±<br>0.010  | 0.441 ±<br>0.008 | 3.416 ±<br>0.024 | 3.156 ±<br>0.024 | 0.960 ±<br>0.009  |
| Marmesin (12)                 | -                 | -                 | -                | -                | -                 | -                | 1.476 ±<br>0.015 | -                 | -                | -                | -                | -                 |
| sec-O-Glucosyl-hamaudol (13)  | 0.201 ±<br>0.012  | 0.254 ±<br>0.006  | 0.092 ±<br>0.002 | 0.106 ±<br>0.002 | 0.094 ±<br>0.001  | 0.070 ±<br>0.003 | -                | 0.387 ±<br>0.010  | 0.652 ±<br>0.009 | -                | -                | 0.298 ±<br>0.003  |
| Oxypeucedanin hydrate (14)    | 4.860 ±<br>0.207  | 6.903 ±<br>0.202  | 0.568 ±<br>0.007 | 0.592 ±<br>0.002 | 5.299 ±<br>0.081  | 0.465 ±<br>0.000 | -                | 11.089 ±<br>0.230 | 4.323 ±<br>0.094 | 0.569 ±<br>0.007 | 0.796 ±<br>0.013 | 7.091 ±<br>0.048  |
| Decursinol (15)               | -                 | -                 | -                | -                | -                 | -                | 3.447 ±<br>0.029 | -                 | -                | -                | -                | -                 |
| Psoralen (18)                 | 0.046 ±<br>0.003  | 0.151 ±<br>0.009  | 0.031 ±<br>0.001 | 0.018 ±<br>0.001 | 0.050 ±<br>0.002  | 0.060 ±<br>0.003 | 0.183 ±<br>0.003 | 0.102 ±<br>0.006  | 0.026 ±<br>0.001 | 0.063 ±<br>0.002 | 0.076 ±<br>0.005 | -                 |
| Xanthotoxin (22)              | 0.058 ±<br>0.003  | 0.160 ±<br>0.006  | 0.082 ±<br>0.003 | 0.038 ±<br>0.001 | 0.061 ±<br>0.001  | 0.029 ±<br>0.001 | 0.353 ±<br>0.008 | 0.088 ±<br>0.010  | 0.118 ±<br>0.001 | 0.089 ±<br>0.002 | 0.104 ±<br>0.007 | -                 |
| Bergapten (25)                | 0.437 ±<br>0.022  | 0.312 ±<br>0.010  | 0.131 ±<br>0.003 | 0.157 ±<br>0.000 | 0.256 ±<br>0.003  | 0.073 ±<br>0.004 | 0.206 ±<br>0.006 | 0.328 ±<br>0.003  | 0.133 ±<br>0.004 | 0.132 ±<br>0.001 | 0.182 ±<br>0.002 | -                 |
| Ostenol (26)                  | 2.186 ±<br>0.088  | 3.642 ±<br>0.056  | -                | -                | 3.896 ±<br>0.051  | -                | -                | 3.337 ±<br>0.060  | 1.410 ±<br>0.026 | -                | -                | 3.213 ±<br>0.026  |
| Bisabolangelone (27)          | 9.145 ±<br>0.475  | 27.728 ±<br>0.653 | 9.004 ±<br>0.225 | 7.275 ±<br>0.115 | 3.976 ±<br>0.052  | 2.366 ±<br>0.040 | 0.276 ±<br>0.003 | 2.416 ±<br>0.054  | 0.079 ±<br>0.002 | 3.647 ±<br>0.053 | 9.039 ±<br>0.074 | 5.620 ±<br>0.048  |
| Oxypeucedanin (29)            | 14.602 ±<br>0.639 | 27.543 ±<br>0.540 | 0.155 ±<br>0.002 | 0.135 ±<br>0.001 | 16.158 ±<br>0.231 | 0.089 ±<br>0.009 | -                | 19.512 ±<br>0.393 | 2.381 ±<br>0.053 | 0.146 ±<br>0.002 | 1.159 ±<br>0.006 | 22.302 ±<br>0.141 |
| Columbianetin acetate (30)    | -                 | -                 | -                | -                | -                 | -                | 0.176 ±<br>0.003 | -                 | -                | -                | -                | -                 |
| Coniferyl ferulate (31)       | 1.425 ±<br>0.078  | 5.668 ±<br>0.197  | 1.795 ±<br>0.010 | 1.459 ±<br>0.023 | -                 | -                | -                | -                 | -                | 0.804 ±<br>0.016 | 1.830 ±<br>0.032 | 1.088 ±<br>0.014  |
| Imperatorin (34)              | 1.091 ±<br>0.048  | 6.636 ±<br>0.129  | -                | 0.051 ±<br>0.000 | 0.876 ±<br>0.012  | -                | -                | 5.610 ±<br>0.109  | 1.562 ±<br>0.033 | -                | 0.290 ±<br>0.001 | 6.429 ±<br>0.045  |

|  |                   |                   |                   |                   |                   |                   |                   |                  |                  |                  |                   |                   |
|--|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|------------------|------------------|------------------|-------------------|-------------------|
| Ligustilide ( <b>35</b> )                  | -                 | -                 | -                 | -                 | -                 | -                 | 0.300 ±<br>0.005  | -                | -                | -                | -                 | -                 |
| Osthol ( <b>37</b> )                       | 5.839 ±<br>0.249  | 3.833 ±<br>0.077  | -                 | -                 | 5.290 ±<br>0.071  | -                 | -                 | 5.299 ±<br>0.101 | 8.372 ±<br>0.169 | -                | -                 | 5.597 ±<br>0.036  |
| Decursin ( <b>38</b> )                     | -                 | 3.111 ±<br>0.066  | -                 | -                 | 0.385 ±<br>0.005  | -                 | 68.772 ±<br>0.538 | 0.160 ±<br>0.006 | -                | -                | 1.462 ±<br>0.012  | -                 |
| Decursinol angelate<br>( <b>39</b> )       | -                 | 3.705 ±<br>0.072  | -                 | -                 | 0.347 ±<br>0.005  | -                 | 61.206 ±<br>0.481 | 0.178 ±<br>0.005 | -                | -                | 1.915 ±<br>0.011  | -                 |
| Isoimperatorin ( <b>40</b> )               | 8.041 ±<br>0.347  | 9.150 ±<br>0.194  | 0.309 ±<br>0.008  | 0.510 ±<br>0.005  | 7.319 ±<br>0.096  | 0.314 ±<br>0.001  | -                 | 7.536 ±<br>0.146 | 7.858 ±<br>0.162 | 0.284 ±<br>0.006 | 1.115 ±<br>0.011  | 10.956 ±<br>0.072 |
| Falcarindiol ( <b>43</b> )                 | -                 | 1.949 ±<br>0.016  | 3.043 ±<br>0.032  | 3.608 ±<br>0.031  | 1.207 ±<br>0.016  | 10.695 ±<br>0.128 | -                 | 1.242 ±<br>0.069 | -                | 7.224 ±<br>0.126 | 14.159 ±<br>0.128 | 2.009 ±<br>0.016  |
| Compound                                   | ARE-13            | ARE-14            | ARE-15            | ARE-16            | ARE-17            | ARE-18            | ARE-19            | ARE-20           | ARE-21           | ARE-22           | ARE-23            | ARE-24            |
| Chlorogenic acid ( <b>1</b> )              | 13.492 ±<br>0.210 | 12.593 ±<br>0.244 | 16.356 ±<br>0.278 | 12.927 ±<br>0.100 | 11.994 ±<br>0.226 | 5.974 ±<br>0.227  | 7.073 ±<br>0.043  | 4.864 ±<br>0.039 | 6.395 ±<br>0.171 | 6.157 ±<br>0.050 | 12.764 ±<br>0.486 | 10.064 ±<br>0.299 |
| Caffeic acid ( <b>2</b> )                  | 0.153 ±<br>0.002  | 0.203 ±<br>0.007  | 0.361 ±<br>0.005  | 0.238 ±<br>0.012  | 0.259 ±<br>0.006  | 0.174 ±<br>0.006  | 0.136 ±<br>0.002  | 0.265 ±<br>0.003 | 0.117 ±<br>0.001 | 0.247 ±<br>0.003 | 0.308 ±<br>0.008  | 0.500 ±<br>0.008  |
| Prim-O-glucosyl-<br>cimifugin ( <b>3</b> ) | 3.778 ±<br>0.031  | 3.616 ±<br>0.053  | 6.535 ±<br>0.026  | 4.701 ±<br>0.063  | 2.787 ±<br>0.005  | -                 | -                 | -                | -                | -                | 3.863 ±<br>0.095  | 4.719 ±<br>0.067  |
| Cimifugin ( <b>4</b> )                     | 0.321 ±<br>0.024  | 1.830 ±<br>0.038  | 1.515 ±<br>0.010  | 1.012 ±<br>0.012  | 1.719 ±<br>0.009  | -                 | -                 | -                | -                | -                | 1.405 ±<br>0.032  | 2.673 ±<br>0.023  |
| Ferulic acid ( <b>7</b> )                  | 0.854 ±<br>0.003  | 0.658 ±<br>0.012  | 0.693 ±<br>0.005  | 0.667 ±<br>0.011  | -                 | -                 | 2.698 ±<br>0.033  | 4.607 ±<br>0.056 | 2.801 ±<br>0.054 | 3.866 ±<br>0.046 | 1.734 ±<br>0.033  | 0.606 ±<br>0.005  |
| Marmesin ( <b>12</b> )                     | -                 | 0.297 ±<br>0.002  | 0.477 ±<br>0.001  | 0.254 ±<br>0.007  | -                 | -                 | -                 | -                | -                | -                | -                 | -                 |
| sec-O-Glucosyl-<br>hamaudol ( <b>13</b> )  | 0.067 ±<br>0.003  | 0.135 ±<br>0.002  | 0.320 ±<br>0.005  | 0.300 ±<br>0.003  | 0.366 ±<br>0.010  | 0.089 ±<br>0.001  | 0.081 ±<br>0.006  | -                | 0.107 ±<br>0.010 | 0.090 ±<br>0.003 | 0.354 ±<br>0.002  | 0.534 ±<br>0.020  |
| Oxypeucedanin<br>hydrate ( <b>14</b> )     | 6.499 ±<br>0.049  | 2.677 ±<br>0.048  | 8.861 ±<br>0.040  | 6.250 ±<br>0.061  | 6.502 ±<br>0.031  | 0.299 ±<br>0.005  | 0.385 ±<br>0.009  | 0.810 ±<br>0.009 | 0.474 ±<br>0.004 | 0.808 ±<br>0.005 | 8.544 ±<br>0.192  | 11.538 ±<br>0.123 |
| Decursinol ( <b>15</b> )                   | -                 | -                 | -                 | -                 | -                 | -                 | -                 | -                | -                | -                | -                 | -                 |
| Psoralen ( <b>18</b> )                     | 0.031 ±<br>0.001  | 0.094 ±<br>0.001  | 0.186 ±<br>0.001  | 0.025 ±<br>0.001  | 0.057 ±<br>0.002  | 0.053 ±<br>0.003  | 0.293 ±<br>0.005  | -                | 0.099 ±<br>0.003 | 0.072 ±<br>0.004 | 0.086 ±<br>0.002  | 0.061 ±<br>0.001  |
| Xanthotoxin ( <b>22</b> )                  | 0.040 ±<br>0.000  | 0.132 ±<br>0.001  | 0.369 ±<br>0.008  | 0.031 ±<br>0.001  | 0.069 ±<br>0.000  | 0.099 ±<br>0.006  | 0.459 ±<br>0.005  | 0.126 ±<br>0.006 | 0.105 ±<br>0.003 | 0.064 ±<br>0.001 | 0.114 ±<br>0.002  | 0.034 ±<br>0.001  |
| Bergapten ( <b>25</b> )                    | 0.222 ±<br>0.001  | 0.132 ±<br>0.001  | 1.758 ±<br>0.015  | 0.255 ±<br>0.004  | 0.254 ±<br>0.002  | -                 | 0.325 ±<br>0.002  | 0.247 ±<br>0.003 | 0.160 ±<br>0.003 | 0.100 ±<br>0.006 | 0.169 ±<br>0.001  | 0.225 ±<br>0.004  |
| Ostenol ( <b>26</b> )                      | 4.453 ±<br>0.022  | 2.229 ±<br>0.022  | 3.908 ±<br>0.034  | 3.045 ±<br>0.016  | 2.313 ±<br>0.008  | -                 | -                 | -                | 0.116 ±<br>0.006 | -                | 3.802 ±<br>0.075  | 4.840 ±<br>0.034  |

|                            |                   |                   |                   |                   |                   |                   |                  |                   |                  |                  |                  |                   |
|----------------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|------------------|-------------------|------------------|------------------|------------------|-------------------|
| Bisabolangelone            | 11.435 ±<br>0.140 | 5.844 ±<br>0.053  | 3.694 ±<br>0.027  | 4.682 ±<br>0.058  | 2.793 ±<br>0.013  | 2.234 ±<br>0.023  | 3.134 ±<br>0.036 | 7.792 ±<br>0.103  | 5.911 ±<br>0.059 | 0.412 ±<br>0.007 | 0.696 ±<br>0.015 | 0.284 ±<br>0.006  |
| Oxypeucedanin (29)         | 22.863 ±<br>0.240 | 9.134 ±<br>0.075  | 20.013 ±<br>0.130 | 14.746 ±<br>0.162 | 13.965 ±<br>0.055 | -                 | 0.104 ±<br>0.005 | -                 | 0.250 ±<br>0.001 | -                | 7.825 ±<br>0.154 | 11.399 ±<br>0.095 |
| Columbianetin acetate (30) | -                 | -                 | -                 | -                 | -                 | -                 | -                | -                 | -                | -                | -                | -                 |
| Coniferyl ferulate (31)    | 1.890 ±<br>0.037  | 1.137 ±<br>0.025  | 0.738 ±<br>0.041  | 1.726 ±<br>0.029  | -                 | 0.454 ±<br>0.019  | 1.356 ±<br>0.022 | 1.393 ±<br>0.021  | 1.612 ±<br>0.047 | -                | -                | -                 |
| Imperatorin (34)           | 3.578 ±<br>0.039  | 0.894 ±<br>0.010  | 5.277 ±<br>0.036  | 2.376 ±<br>0.030  | 2.429 ±<br>0.024  | -                 | 0.038 ±<br>0.003 | 0.118 ±<br>0.001  | -                | 0.127 ±<br>0.001 | 0.691 ±<br>0.036 | 1.740 ±<br>0.014  |
| Ligustilide (35)           | -                 | -                 | -                 | -                 | -                 | -                 | -                | -                 | -                | -                | -                | -                 |
| Osthol (37)                | 5.635 ±<br>0.061  | 4.978 ±<br>0.043  | 6.384 ±<br>0.035  | 6.929 ±<br>0.072  | 5.189 ±<br>0.009  | -                 | -                | -                 | -                | -                | 8.220 ±<br>0.177 | 7.812 ±<br>0.057  |
| Decursin (38)              | -                 | 15.900 ±<br>0.147 | -                 | 28.824 ±<br>0.344 | 0.163 ±<br>0.001  | -                 | 0.108 ±<br>0.001 | -                 | -                | 0.284 ±<br>0.001 | 0.396 ±<br>0.009 | -                 |
| Decursinol angelate (39)   | -                 | 16.549 ±<br>0.157 | -                 | 22.917 ±<br>0.281 | 0.158 ±<br>0.001  | -                 | -                | -                 | -                | 0.232 ±<br>0.002 | 0.419 ±<br>0.007 | -                 |
| Isoimperatorin (40)        | 7.205 ±<br>0.086  | 3.275 ±<br>0.032  | 19.996 ±<br>0.130 | 3.546 ±<br>0.043  | 7.795 ±<br>0.028  | 0.322 ±<br>0.005  | 0.292 ±<br>0.004 | 0.874 ±<br>0.014  | 0.306 ±<br>0.004 | 0.559 ±<br>0.003 | 5.019 ±<br>0.114 | 6.554 ±<br>0.051  |
| Falcarindiol (43)          | 1.027 ±<br>0.037  | -                 | 1.867 ±<br>0.018  | 1.426 ±<br>0.012  | 1.235 ±<br>0.022  | 12.221 ±<br>0.204 | 4.752 ±<br>0.016 | 15.942 ±<br>0.171 | 9.572 ±<br>0.100 | 6.193 ±<br>0.052 | 2.312 ±<br>0.038 | 0.660 ±<br>0.021  |

ARE, *A.reflexa*. The amounts of the marker compounds are expressed as 'Mean ± standard deviation'.

**Table S13.** Mean amounts of the marker compounds in the methanol extracts of *A. sinensis* samples (mg/g)

| Compound                          | ASI-01         | ASI-02         | ASI-03        | ASI-04         | ASI-05         | ASI-06         | ASI-07        | ASI-08         | ASI-09         | ASI-10         | ASI-11         | ASI-12         |
|-----------------------------------|----------------|----------------|---------------|----------------|----------------|----------------|---------------|----------------|----------------|----------------|----------------|----------------|
| Chlorogenic acid ( <b>1</b> )     | 0.677 ± 0.033  | 0.371 ± 0.022  | 4.514 ± 0.182 | 0.337 ± 0.024  | 0.595 ± 0.053  | 0.641 ± 0.024  | 3.385 ± 0.099 | 0.338 ± 0.010  | 0.251 ± 0.005  | 1.214 ± 0.054  | 0.416 ± 0.017  | 0.376 ± 0.012  |
| Caffeic acid ( <b>2</b> )         | 0.047 ± 0.005  | 0.031 ± 0.004  | 0.114 ± 0.015 | 0.024 ± 0.004  | 0.030 ± 0.004  | 0.044 ± 0.002  | 0.088 ± 0.004 | 0.042 ± 0.002  | 0.023 ± 0.002  | 0.071 ± 0.003  | 0.048 ± 0.003  | 0.024 ± 0.002  |
| Ferulic acid ( <b>7</b> )         | 2.209 ± 0.039  | 1.388 ± 0.011  | 1.163 ± 0.006 | 1.854 ± 0.019  | 1.978 ± 0.026  | 2.198 ± 0.051  | 0.747 ± 0.004 | 1.576 ± 0.013  | 1.853 ± 0.005  | 2.133 ± 0.046  | 2.055 ± 0.036  | 2.216 ± 0.024  |
| Benzoic acid ( <b>8</b> )         | 0.068 ± 0.003  | 0.043 ± 0.003  | 0.056 ± 0.007 | 0.049 ± 0.002  | 0.070 ± 0.006  | 0.064 ± 0.001  | 0.041 ± 0.003 | 0.048 ± 0.003  | 0.056 ± 0.001  | 0.093 ± 0.006  | 0.073 ± 0.003  | 0.045 ± 0.002  |
| Senkyunolide I ( <b>9</b> )       | 2.296 ± 0.070  | 1.699 ± 0.032  | 1.808 ± 0.033 | 2.526 ± 0.023  | 2.972 ± 0.046  | 3.088 ± 0.084  | 1.455 ± 0.013 | 1.411 ± 0.026  | 3.237 ± 0.004  | 3.168 ± 0.094  | 4.131 ± 0.069  | 3.114 ± 0.046  |
| Senkyunolide H ( <b>11</b> )      | 0.416 ± 0.016  | 0.304 ± 0.007  | 0.357 ± 0.008 | 0.477 ± 0.006  | 0.530 ± 0.008  | 0.546 ± 0.016  | 0.263 ± 0.003 | 0.274 ± 0.006  | 0.592 ± 0.007  | 0.577 ± 0.019  | 0.742 ± 0.014  | 0.568 ± 0.009  |
| Senkyunolide A ( <b>32</b> )      | 0.404 ± 0.014  | 0.423 ± 0.029  | 0.574 ± 0.005 | 0.597 ± 0.008  | 0.464 ± 0.009  | 0.369 ± 0.020  | 0.442 ± 0.005 | 0.694 ± 0.014  | 0.416 ± 0.011  | 0.974 ± 0.028  | 0.586 ± 0.033  | 0.532 ± 0.012  |
| 3-n-Butyl-phthalide ( <b>33</b> ) | 0.435 ± 0.005  | 0.520 ± 0.004  | 0.150 ± 0.003 | 0.547 ± 0.007  | 0.363 ± 0.005  | 0.506 ± 0.009  | 0.164 ± 0.004 | 0.142 ± 0.001  | 0.508 ± 0.004  | 0.750 ± 0.015  | 0.779 ± 0.012  | 0.474 ± 0.004  |
| Ligustilide ( <b>35</b> )         | 30.033 ± 0.855 | 11.175 ± 0.207 | 8.616 ± 0.155 | 20.379 ± 0.191 | 32.023 ± 0.447 | 27.501 ± 0.715 | 6.402 ± 0.029 | 46.474 ± 0.834 | 22.380 ± 0.059 | 36.554 ± 1.038 | 18.361 ± 0.307 | 23.464 ± 0.331 |
| Falcarindiol ( <b>43</b> )        | 2.044 ± 0.088  | 0.723 ± 0.049  | 8.880 ± 0.128 | 1.490 ± 0.037  | 1.546 ± 0.016  | 1.987 ± 0.027  | 5.843 ± 0.191 | 2.627 ± 0.034  | 1.377 ± 0.027  | 1.624 ± 0.056  | 1.306 ± 0.028  | 1.588 ± 0.031  |
| Levistilide A ( <b>45</b> )       | 5.286 ± 0.178  | 1.866 ± 0.030  | 2.499 ± 0.047 | 1.701 ± 0.013  | 3.367 ± 0.060  | 5.295 ± 0.156  | 1.479 ± 0.020 | 1.971 ± 0.034  | 2.825 ± 0.015  | 2.693 ± 0.075  | 2.220 ± 0.037  | 2.266 ± 0.026  |

ASI, *A. sinensis*. The amounts of the marker compounds are expressed as ‘Mean ± standard deviation’.

**Table S14.** Mean amounts of the marker compounds in the methanol extracts of *Conioselinum tenuissimum* samples (mg/g)

| Compound                          | CTE-01         | CTE-02         | CTE-03         | CTE-04         | CTE-05         | CTE-06         | CTE-07         | CTE-08          |
|-----------------------------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|-----------------|
| Chlorogenic acid ( <b>1</b> )     | 1.128 ± 0.019  | 2.125 ± 0.039  | 3.062 ± 0.070  | 2.533 ± 0.045  | 2.775 ± 0.020  | 3.723 ± 0.077  | 2.488 ± 0.016  | 1.053 ± 0.008   |
| Caffeic acid ( <b>2</b> )         | 0.035 ± 0.001  | 0.053 ± 0.001  | 0.071 ± 0.001  | 0.049 ± 0.001  | 0.065 ± 0.002  | 0.036 ± 0.000  | 0.048 ± 0.000  | -               |
| Ferulic acid ( <b>7</b> )         | 1.028 ± 0.005  | 0.847 ± 0.009  | 1.184 ± 0.015  | 1.090 ± 0.015  | 0.926 ± 0.006  | 1.236 ± 0.010  | 0.574 ± 0.006  | 0.620 ± 0.015   |
| Benzoic acid ( <b>8</b> )         | 0.069 ± 0.002  | 0.225 ± 0.004  | 0.056 ± 0.003  | 0.049 ± 0.002  | 0.038 ± 0.001  | 0.032 ± 0.002  | 0.125 ± 0.002  | -               |
| Senkyunolide I ( <b>9</b> )       | 2.434 ± 0.019  | 3.834 ± 0.051  | 3.196 ± 0.043  | 2.334 ± 0.034  | 2.104 ± 0.017  | 2.324 ± 0.027  | 3.902 ± 0.033  | 0.894 ± 0.003   |
| Senkyunolide H ( <b>11</b> )      | 0.419 ± 0.004  | 0.536 ± 0.010  | 0.545 ± 0.008  | 0.384 ± 0.009  | 0.331 ± 0.003  | 0.377 ± 0.005  | 0.614 ± 0.013  | 0.155 ± 0.001   |
| Bergapten ( <b>25</b> )           | -              | -              | -              | -              | -              | -              | -              | -               |
| Bisabolangelone ( <b>27</b> )     | 0.086 ± 0.001  | -              | -              | -              | -              | -              | -              | -               |
| Coniferyl ferulate ( <b>31</b> )  | 3.272 ± 0.046  | 0.248 ± 0.008  | 4.456 ± 0.095  | 4.966 ± 0.093  | 4.579 ± 0.074  | 9.532 ± 0.188  | 0.925 ± 0.009  | 8.968 ± 0.197   |
| Senkyunolide A ( <b>32</b> )      | 1.272 ± 0.014  | -              | 2.118 ± 0.030  | 1.504 ± 0.023  | 1.110 ± 0.010  | 9.612 ± 0.113  | 3.285 ± 0.027  | 2.328 ± 0.016   |
| 3-n-Butyl-phthalide ( <b>33</b> ) | 0.855 ± 0.007  | 1.292 ± 0.017  | 0.576 ± 0.006  | 0.496 ± 0.007  | 0.357 ± 0.002  | 1.140 ± 0.016  | 1.497 ± 0.009  | 0.294 ± 0.003   |
| Ligustilide ( <b>35</b> )         | 37.908 ± 0.270 | 11.013 ± 0.151 | 76.923 ± 1.056 | 63.354 ± 0.892 | 61.766 ± 0.482 | 58.015 ± 0.644 | 21.749 ± 0.174 | 110.078 ± 0.628 |
| Falcarindiol ( <b>43</b> )        | 0.603 ± 0.012  | -              | 1.285 ± 0.037  | 1.355 ± 0.024  | 1.415 ± 0.016  | 1.440 ± 0.050  | -              | 2.708 ± 0.048   |
| Levistilide A ( <b>45</b> )       | 3.853 ± 0.042  | 8.900 ± 0.116  | 6.863 ± 0.103  | 6.712 ± 0.118  | 5.775 ± 0.059  | 4.811 ± 0.068  | 6.918 ± 0.064  | 3.228 ± 0.028   |

CTE, *Conioselinum tenuissimum*. The amounts of the marker compounds are expressed as ‘Mean ± standard deviation’.

**Table S15.** Mean amounts of the marker compounds in the methanol extracts of *Ostericum grosserratum* samples (mg/g)

| Compound                | OGR-01             | OGR-02             | OGR-03             | OGR-04             | OGR-05             | OGR-06             | OGR-07              | OGR-08             |
|-------------------------|--------------------|--------------------|--------------------|--------------------|--------------------|--------------------|---------------------|--------------------|
| Chlorogenic acid<br>(1) | -                  | 0.270 ± 0.001      | 0.400 ± 0.004      | 0.280 ± 0.012      | 0.634 ± 0.012      | 0.264 ± 0.002      | 0.327 ± 0.011       | 0.383 ± 0.010      |
| Ferulic acid (7)        | -                  | 0.142 ± 0.002      | 0.257 ± 0.000      | 0.065 ± 0.001      | 0.230 ± 0.009      | 0.195 ± 0.001      | -                   | 0.173 ± 0.006      |
| Psoralen (18)           | 0.049 ± 0.000      | -                  | -                  | -                  | -                  | -                  | -                   | -                  |
| Xanthotoxin (22)        | 0.041 ± 0.000      | -                  | -                  | -                  | -                  | -                  | -                   | -                  |
| Falcarindiol (43)       | 253.520 ±<br>4.443 | 304.869 ±<br>1.630 | 277.503 ±<br>1.905 | 355.783 ±<br>7.968 | 305.420 ±<br>4.119 | 432.044 ±<br>3.455 | 370.395 ±<br>11.298 | 209.759 ±<br>6.517 |

OGR, *Ostericum grosserratum*. The amounts of the marker compounds are expressed as 'Mean ± standard deviation'