









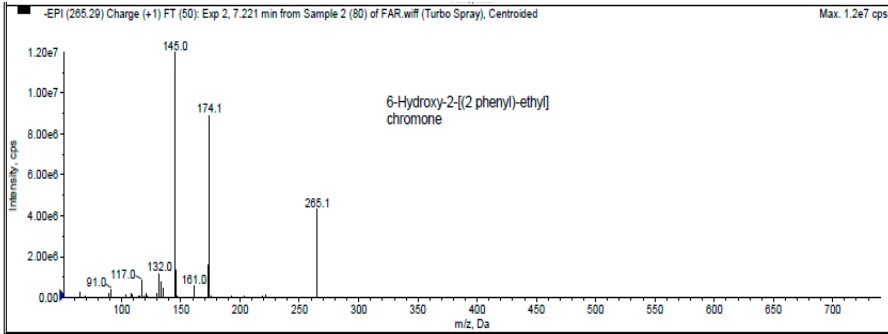
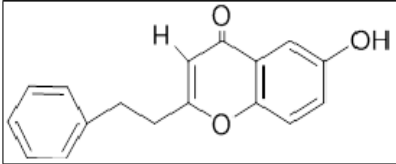
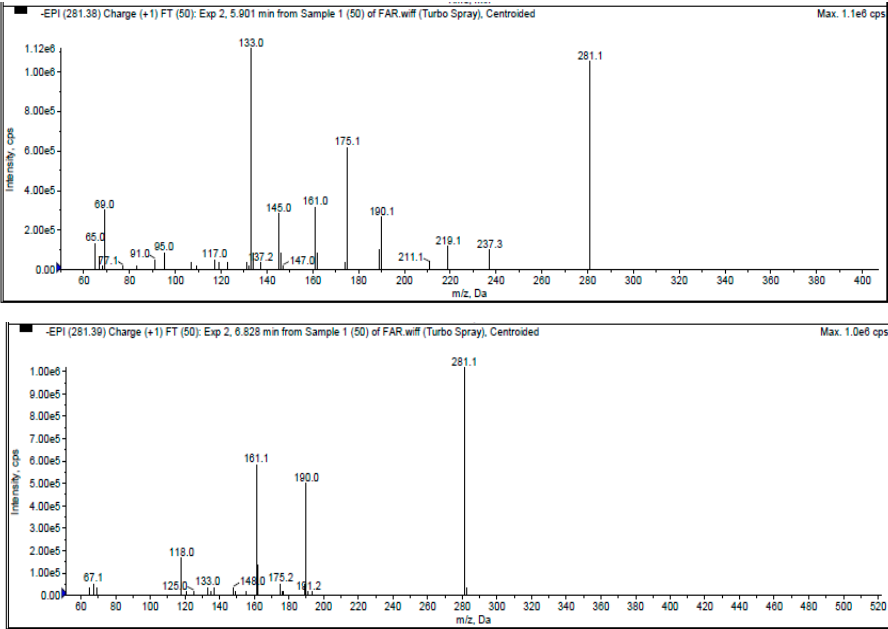
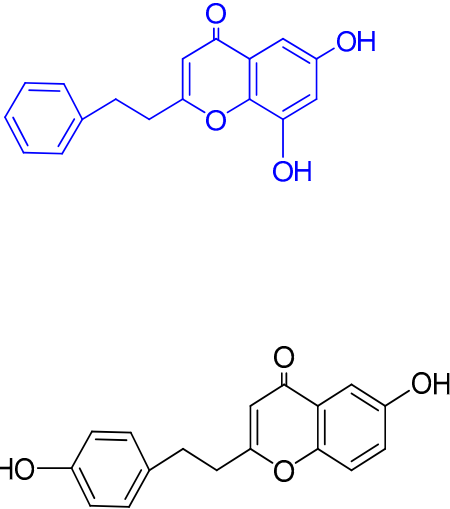
Supplementary information

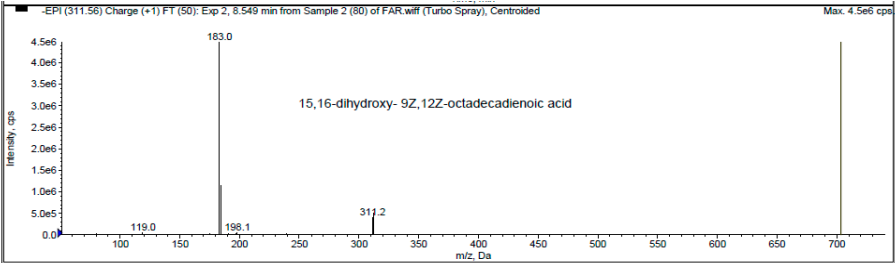
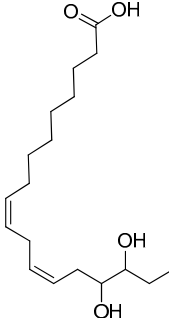
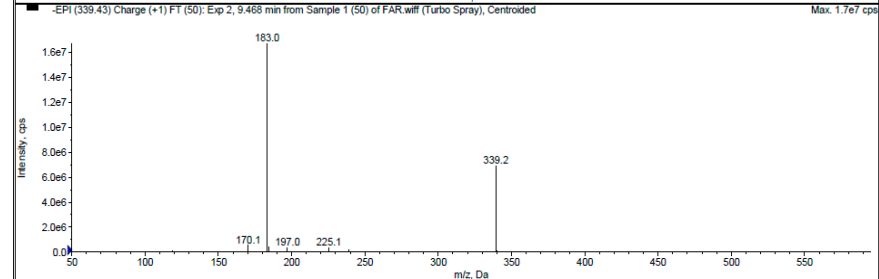
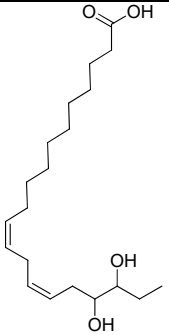
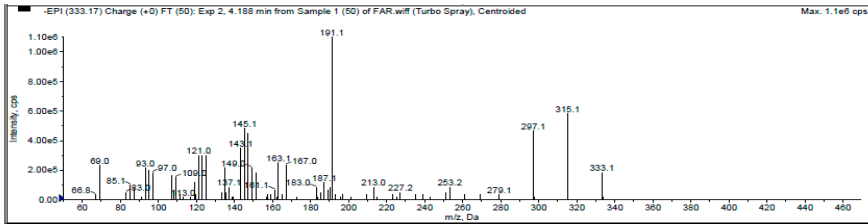
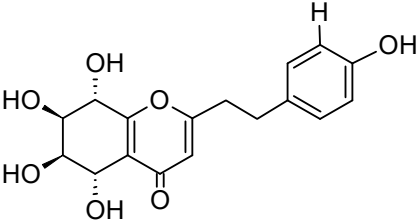
Supplementary Table 1. *A. malaccensis* gaharu samples analysed in the present study. The samples were obtained from traders in Malaysia.

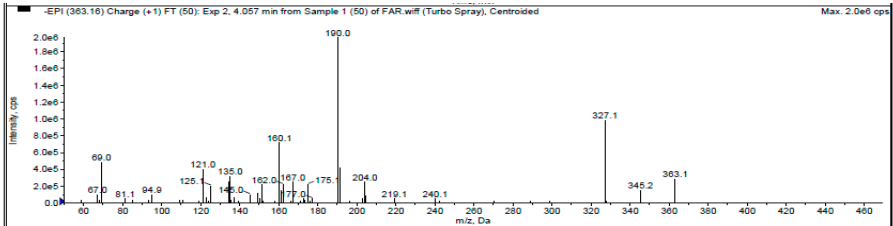
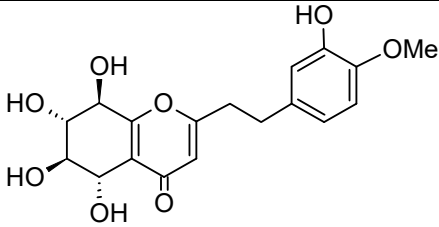
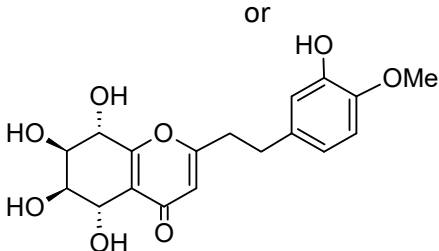
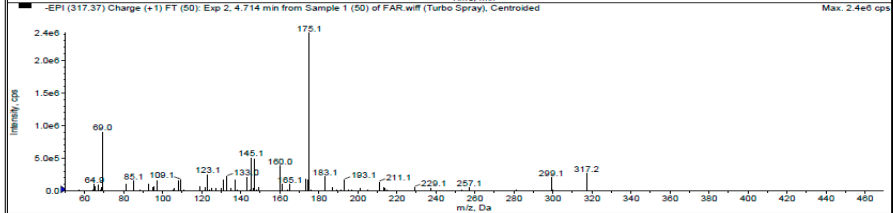
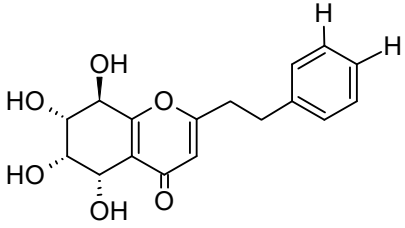
| Label in this study | Market label | Sample image | Price (RM/kg) |
|---------------------|-----------------------|--|---------------|
| A | Kayu AAA - high grade |  | 25,000 |
| B | Kayu A - high grade |  | 20,000 |
| C | Teras |  | 18,000 |
| D | Kayu A - small |  | 16,000 |
| E | Kayu B - high grade |  | 12,000 |

| Label in this study | Market label | Sample image | Price (RM/kg) |
|---------------------|------------------------|--|---------------|
| F | Kayu A - medium |  | 10,000 |
| G | Kayu A - hancur |  | 9,000 |
| H | Teras |  | 2,000 |

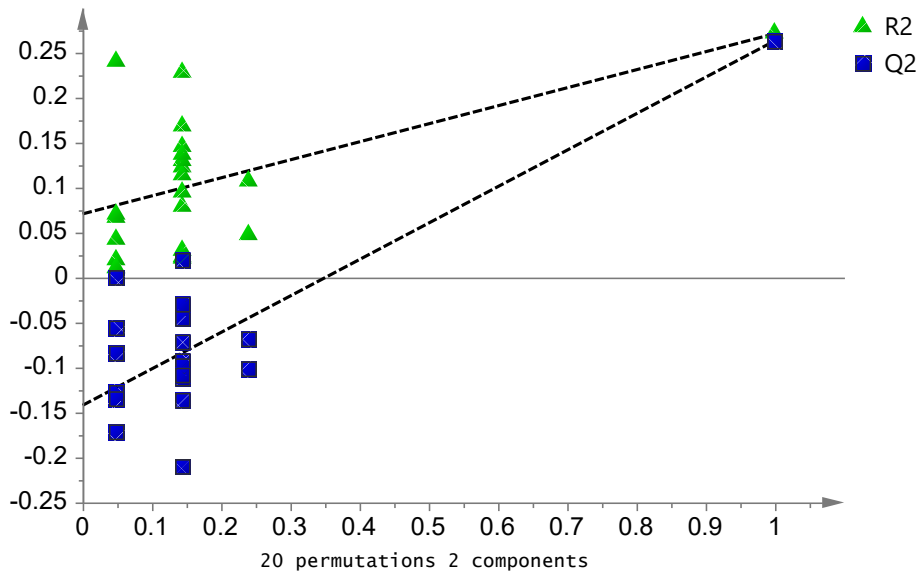
Supplementary Table. 2. LC-MS data of identified metabolites in eight gaharu samples.

| No | Compound name | m/z | structure |
|----|---|---|--|
| 1 | 6- or 7-hydroxy-2-[(2-phenyl)-ethyl]chromone (C ₁₇ H ₁₄ O ₃) | <p>[M-H]⁻ ion at m/z value of 265</p>  |  |
| 2 | 2 isomers of dihydroxy-2-[(2-phenyl)-ethyl]chromones | <p>m/z values of 281</p>  |  |

| | | | |
|---|---|---|---|
| 3 | (9Z,12Z)-15,16-dihydroxyoctadeca-9,12-octadecadienoic acid | <p>[M-H]⁻ ion of m/z 311</p>  |  |
| 4 | (11Z,14Z)-17,18-dihydroxyicosa-11,14-dienoic acid (m/z 340, C ₂₀ H ₃₆ O ₄), | <p>[M-H]⁻ ion at m/z 339</p>  |  |
| 5 | aquilarone F | <p>[M-H]⁻ ions of m/z 333</p>  |  |

| | | | |
|---|-------------------|--|--|
| 6 | aquilarone D or E | <p>[M-H]⁻ ions of m/z 363</p>  <p>Mass spectrum showing intensity (cps) versus m/z (Da) for the [M-H]⁻ ions of m/z 363. The base peak is at m/z 199.0. Other labeled peaks include 69.0, 87.0, 81.1, 94.9, 125.0, 135.0, 145.0, 162.0, 167.0, 175.0, 204.0, 219.1, 240.1, 327.1, 345.2, and 363.1.</p> |  <p>Chemical structure of aquilarone D or E, showing a chromane core with a 3,4-dihydroxyphenyl group at position 2 and a 3,4-dihydroxyphenyl group at position 7. The 7-position phenyl ring has a methoxy group (OMe) at the 3-position.</p> <p>or</p>  <p>Chemical structure of aquilarone B, showing a chromane core with a 3,4-dihydroxyphenyl group at position 2 and a 3,4-dihydroxyphenyl group at position 7. The 7-position phenyl ring has a methoxy group (OMe) at the 3-position.</p> |
| 7 | aquilarone B | <p>[M-H]⁻ ions of m/z 317</p>  <p>Mass spectrum showing intensity (cps) versus m/z (Da) for the [M-H]⁻ ions of m/z 317. The base peak is at m/z 175.1. Other labeled peaks include 64.0, 69.0, 85.1, 109.1, 123.1, 133.0, 145.1, 169.0, 183.1, 193.1, 211.1, 229.1, 257.1, 299.1, and 317.2.</p> |  <p>Chemical structure of aquilarone B, showing a chromane core with a 3,4-dihydroxyphenyl group at position 2 and a 3,4-dihydroxyphenyl group at position 7. The 7-position phenyl ring has two hydrogen atoms (H) at the 3 and 4 positions.</p> |

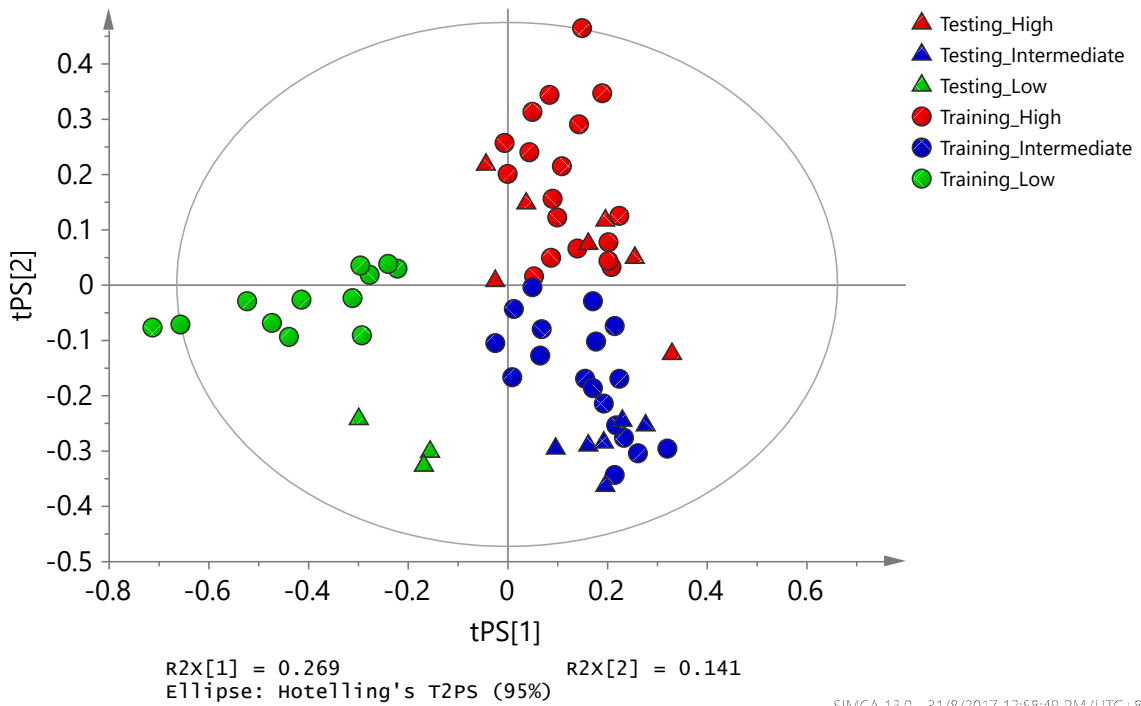
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3 **Supplementary Fig. 1** Permutation test results for the PLS-DA model developed for the
4 *Aquilaria gaharu* samples

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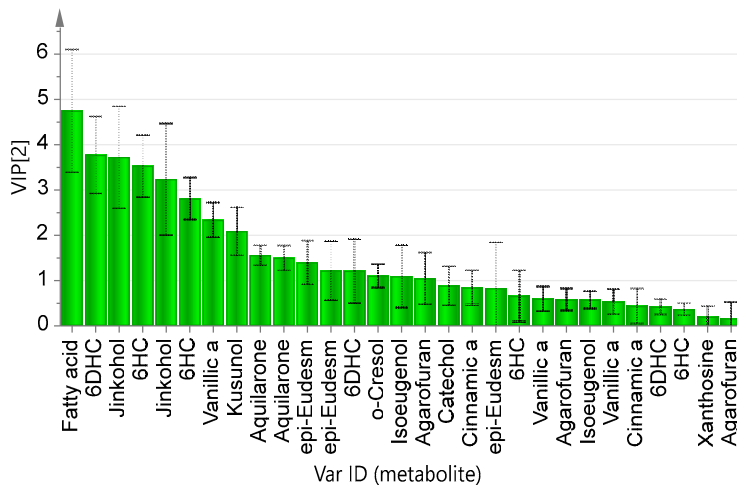


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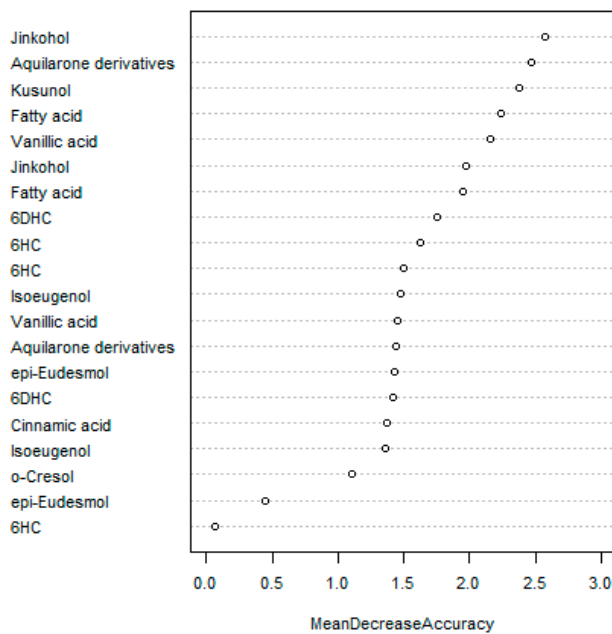
7 **Supplementary Fig 2.** PLSDA score plot of training and testing datasets of three (high,
 8 intermediate, and low) grades of gaharu samples.

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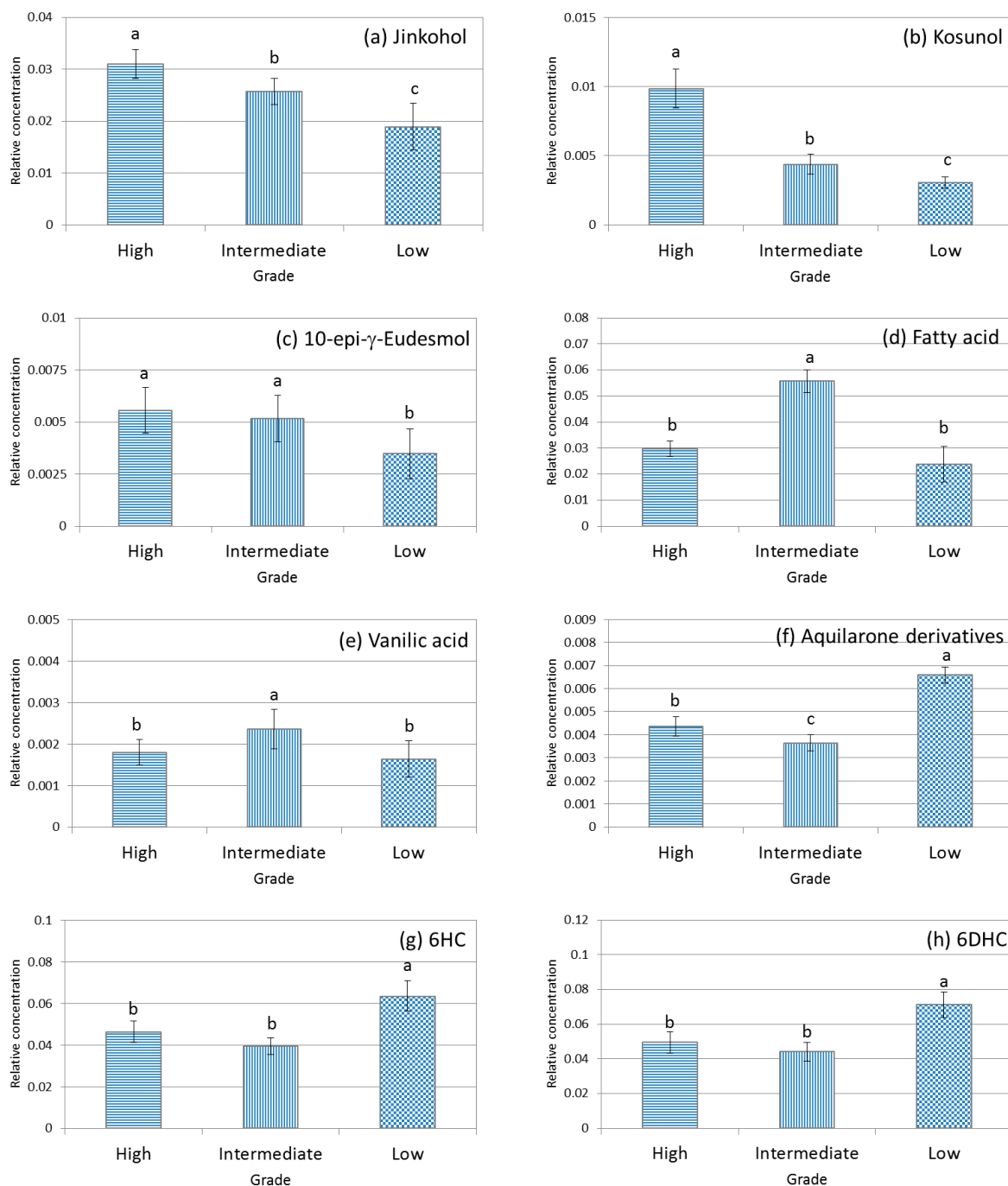
(A) VIP values for PLS-DA



(B) VIP values for Random Forests



10 **Supplementary Fig 3** Variable importance (VIP) values for (a) PLS-DA and (b) Random
 11 Forests models



13 **Supplementary Fig. 4** Relative quantification and statistical analysis for eight chemical
 14 markers: (a) jinkohol, (b) kosunol, (c) 10-epi- γ -eudesmol, (d) fatty acid, (e) vanilic acid, (f)
 15 aquilarone derivatives, (g) 6-hydroxy-2-(2-phenylethyl)chromone (6HC) and (h) 6-hydroxy-2-[2-
 16 (4-hydroxyphenyl)ethyl]chromone (6DHC) for high, intermediate, and low grade groups.

