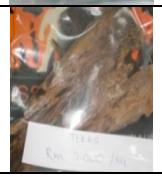
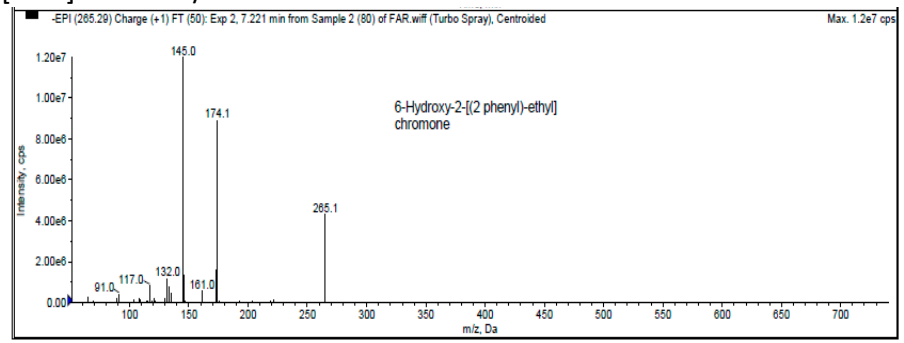
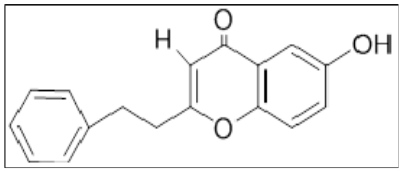
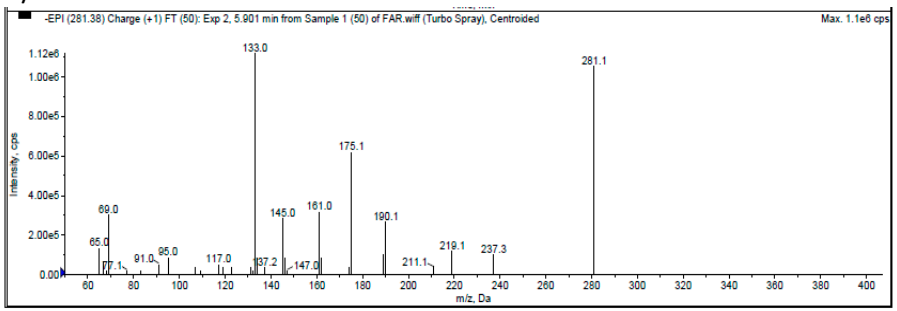
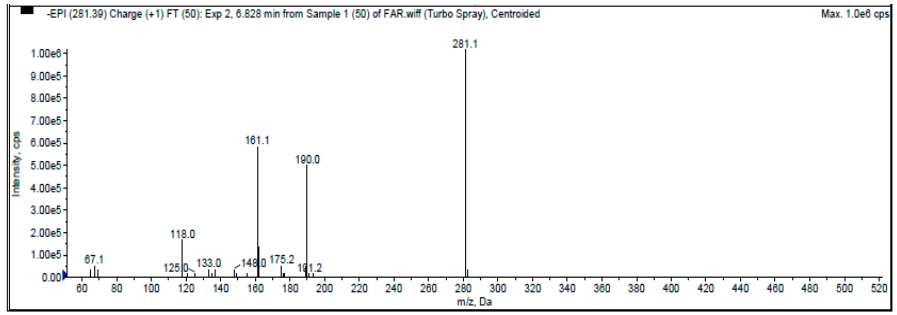
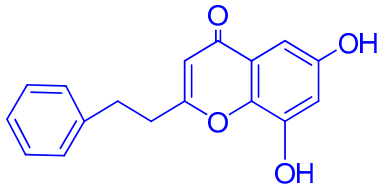
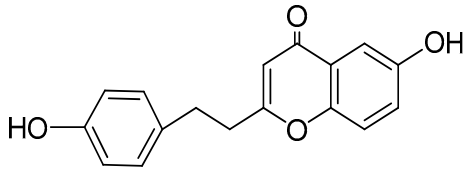
Supplementary information

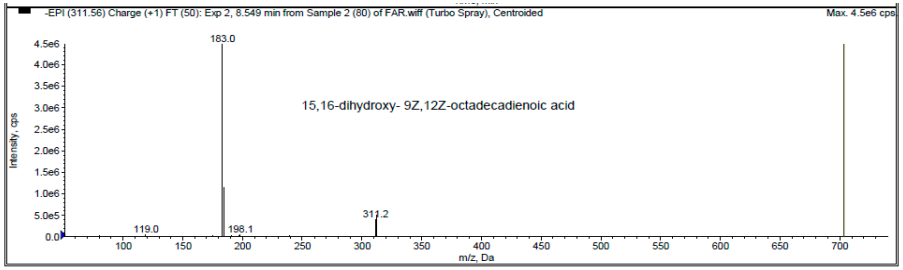
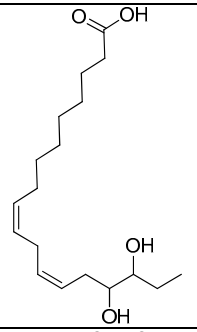
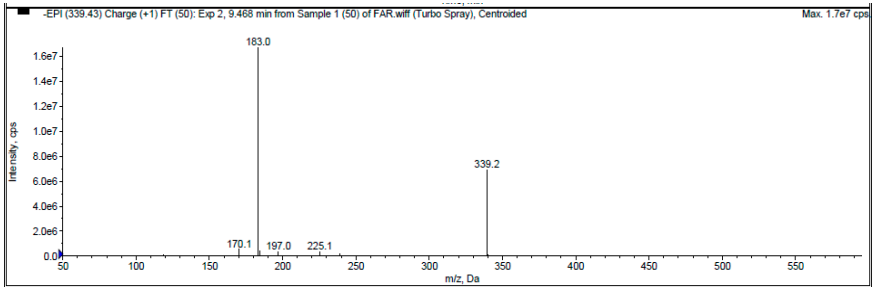
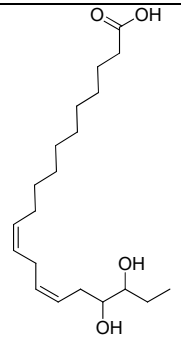
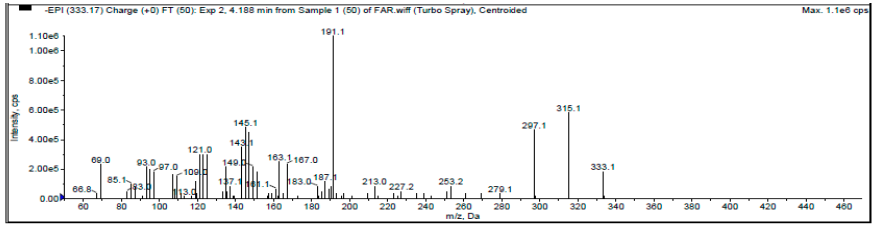
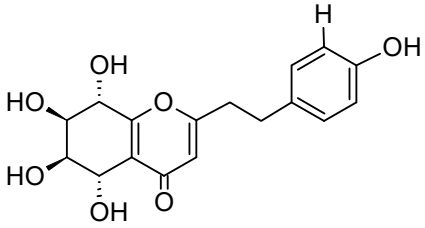
Supplementary Table 1. *A. malaccensis* gaharu samples analysed in the present study. The samples were obtained from traders in Malaysia.

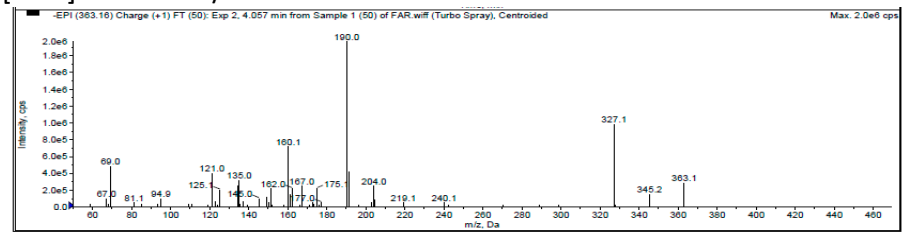
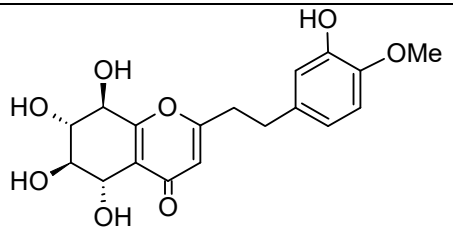
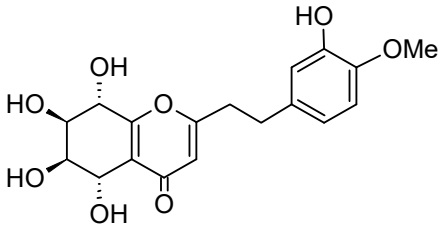
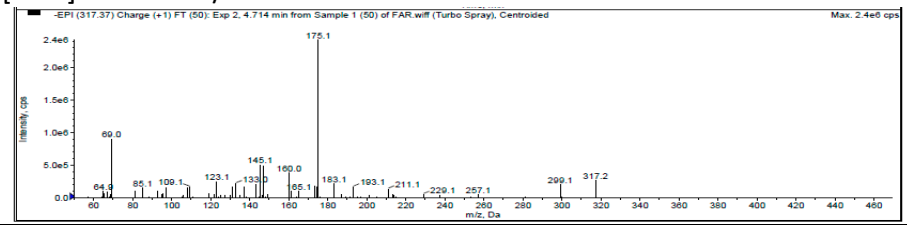
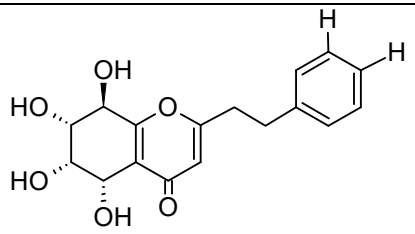
Label in this study	Market label	Sample image	Price (RM/kg)
A	**Kayu AAA - high grade**		**25,000**
B	**Kayu A - high grade**		**20,000**
C	**Teras**		**18,000**
D	**Kayu A - small**		**16,000**
E	**Kayu B - high grade**		**12,000**

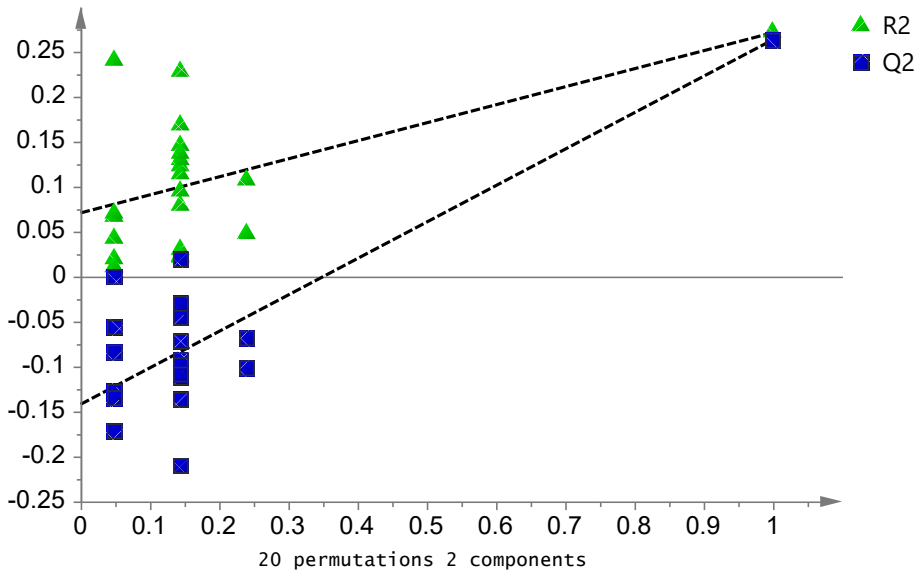
Label in this study	Market label	Sample image	Price (RM/kg)
F	Kayu A - medium		10,000
G	Kayu A - hancur		9,000
H	Teras		2,000

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

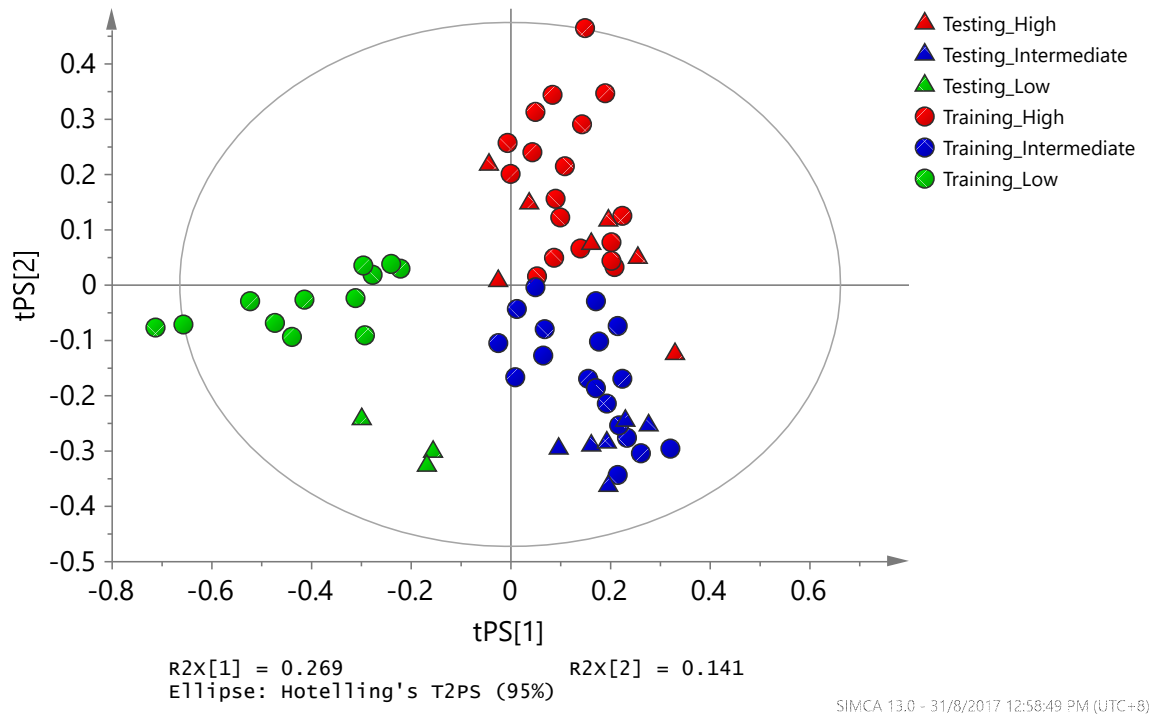
No	Compound name	m/z	structure
1	6- or 7-hydroxy-2-[(2-phenyl)-ethyl]chromone ($C_{17}H_{14}O_3$	[M-H]$^-$ ion at m/z value of 265 	
2	2 isomers of dihydroxy-2-[(2-phenyl)-ethyl]chromones	m/z values of 281  	 

3	(*9Z,12Z*)-15,16-dihydroxyoctadeca-9,12-octadecadienoic acid	[M-H]$^-$ ion of m/z 311 	
4	(*11Z,14Z*)-17,18-dihydroxyicosa-11,14-dienoic acid (m/z 340, $C_{20}H_{36}O_4$),	[M-H]$^-$ ion at m/z 339 	
5	aquilarone F	[M-H]$^-$ ions of m/z 333 	

6	aquilarone D or E	[M-H]⁻ ions of m/z 363  	 or 
7	aquilarone B	[M-H]⁻ ions of m/z 317  	

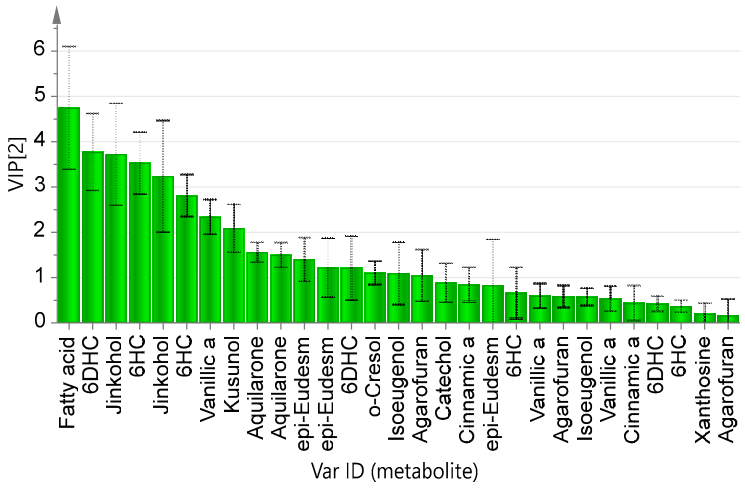


Supplementary Fig. 1 Permutation test results for the PLS-DA model developed for the *Aquilaria* gaharu samples

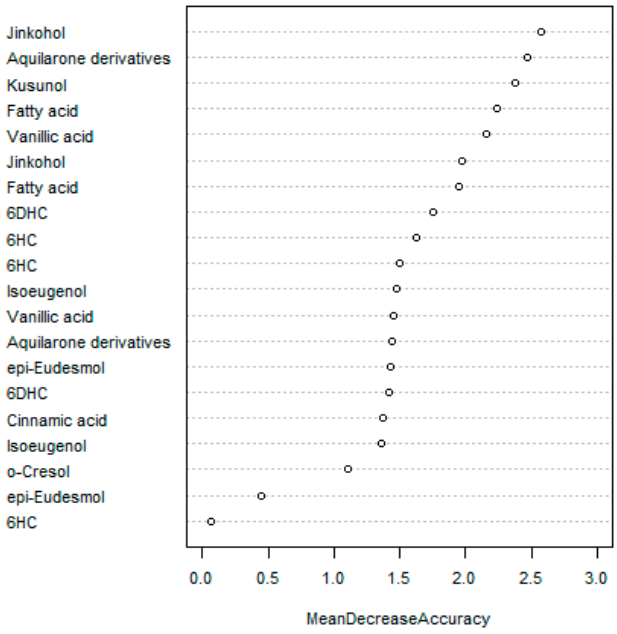


Supplementary Fig 2. PLSDA score plot of training and testing datasets of three (high, intermediate, and low) grades of gaharu samples.

(A) VIP values for PLS-DA



(B) VIP values for Random Forests



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

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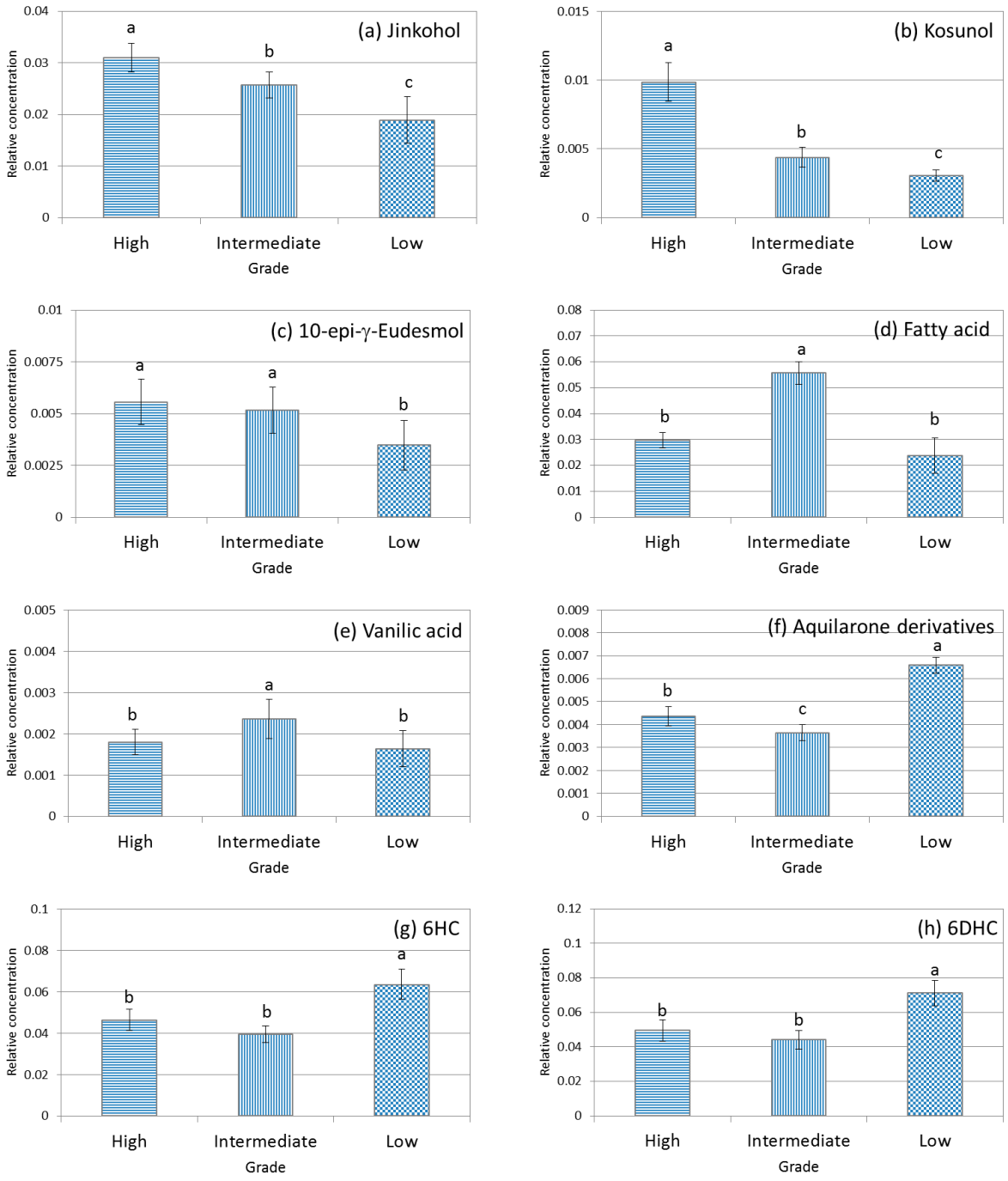

13 **Supplementary Fig. 4** Relative quantification and statistical analysis for eight chemical
14 markers: (a) jinkohol, (b) kosunol, (c) 10-epi-γ-eudesmol, (d) fatty acid, (e) vanilic acid, (f)
15 aquilarone derivatives, (g) 6-hydroxy-2-(2-phenylethyl)chromone (6HC) and (h) 6-hydroxy-2-[2-
16 (4-hydroxyphenyl)ethyl]chromone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