

Supplementary Materials

Table S1. Origin of the different species of cinnamon barks used in the analysis.

Name	Location	Sample codes
<i>Cinnamomum cassia</i>	Malaysia (Kuala Lumpur)	CC
<i>Cinnamomum iners</i>	Malaysia (Kuala Lumpur)	CI
<i>Cinnamomum tamala</i>	Pakistan (Karachi)	CT
<i>Cinnamomum verum</i>	Pakistan (Karachi)	CV
<i>Cinnamomum verum</i>	Malaysia (Kuala Lumpur)	CVM

Table S2. Relative quantification of the most discriminatory metabolites in the studied *Cinnamomum* species identified by UPLC-ESI-MS and multivariate analysis. Values are represented as average ($n=3$) of normalized peak areas $\times 10^3$ to umbelliferon (internal standard) \pm standard error. Different letters indicate significant differences between cinnamon accessions according to least significant difference analysis ($p < 0.05$; Tukey's test).

No.	Rt(min)	Identification	CC ^(a)	CI ^(b)	CT ^(c)	CV ^(d)	CVM ^(e)
1	1.82	Protocatechuic acid	46.46 \pm 0.79 ^{b,c,e}	302.42 \pm 5.67 ^{a,c,d,e}	1110.37 \pm 26.36 ^{a,b,d,e}	3.49 \pm 3.84 ^{b, c, e}	180.3 \pm 3.6 ^{a,b,c,d}
2	3.55	Norboldine	40.27 \pm 1.79 ^b	10078.11 \pm 130.36 ^{a,c,d,e}	6.51 \pm 0.01 ^b	5.71 \pm 1.19 ^b	44.42 \pm 1.88 ^b
3	3.64	Dihydrocinnacasside- <i>O</i> -pentoside	00 \pm 00 ^{b,c,d,e}	29.54 \pm 0.42 ^{a,c,d,e}	366.53 \pm 5.15 ^{a,b,d,e}	13.71 \pm 0.55 ^{a,b,c,e}	26.37 \pm 1.18 ^{a,b,c,d}
4	3.67	Dihydro coumaroyl - <i>O</i> - hexoside	276.51 \pm 10 ^{b,c,d,e}	00 \pm 00 ^{a,c,d}	307.53 \pm 11.72 ^{a,b,d,e}	35.23 \pm 2.01 ^{a,b,c,e}	10.94 \pm 10.01 ^{a,c,d}
5	5.32	Coumarin	1258.21 \pm 10.34 ^d	336.2 \pm 13.21 ^{d,e}	2114.18 \pm 30.25 ^d	947.48 \pm 20.85 ^{a,b,c}	947.9 \pm 10 ^b
6	6.13	Cinnamic acid	30.62 \pm 2.01 ^{b,c,d,e}	124.98 \pm 23.18 ^{a,d,e}	129.85 \pm 15.85 ^{a,d,e}	1120.86 \pm 30.78 ^{a,b,c,e}	1917.9 \pm 7.29 ^{a,b,c,d}
7	6.5	(<i>E</i>)- Cinnamaldehyde	4.92 \pm 1.29 ^{b,d,e}	1413.8 \pm 38.29 ^{a,c,d,e}	52.3 \pm 6.19 ^{b,d,e}	3424.28 \pm 6.84 ^{a,b,c,e}	3831.26 \pm 8.49 ^{a,b,c,d}
8	7.15	Methylcinnamic acid	00 \pm 00 ^{d,e}	226.9 \pm 5.36 ^{d,e}	00 \pm 00 ^{d,e}	13745.3 \pm 18.59 ^{a,b,c,e}	6390.19 \pm 15.96 ^{a,b,c,d}
9	9.00	Methylenedioxy-dimethylepicatechin	5.97 \pm 3.81 ^{b,c,d,e}	78.49 \pm 2.19 ^{a,c,e}	00 \pm 00 ^{a,b,d,e}	78.64 \pm 15.28 ^{a,c,e}	113.59 \pm 5.61 ^{a,b,c,d}
10	14.54	Linoleic acid	221.18 \pm 7.09 ^{b,c,d,e}	2737.3 \pm 51.69 ^{a,c,d,e}	473.19 \pm 15.49 ^{a,b,d,e}	2065.69 \pm 6.28 ^{a,b,c,e}	4371.19 \pm 4.59 ^{a,b,c,d}
11	15.25	Palmitic acid	156.09 \pm 5.49 ^{b,c,d,e}	4340.74 \pm 8.69 ^{a,c,d,e}	616.21 \pm 10.89 ^{a,b,d,e}	4478.69 \pm 3.19 ^{a,b,c,e}	1224.68 \pm 20.49 ^{a,b,c,d}
12	15.54	Oleic acid	122.67 \pm 0.04 ^{b,c,d,e}	1889.67 \pm 8.36 ^{a,c,d}	655.4 \pm 10.59 ^{a,b,d,e}	6391.06 \pm 8.036 ^{a,b,c,e}	1993.61 \pm 3.19 ^{a,c,d}

* CC: *Cinnamomum cassia* from Malaysia, CI: *C. iners* from Malaysia, CT: *C. tamala* from Pakistan, CV: *C. verum* from Pakistan, CVM: *C. verum* from Malaysia.

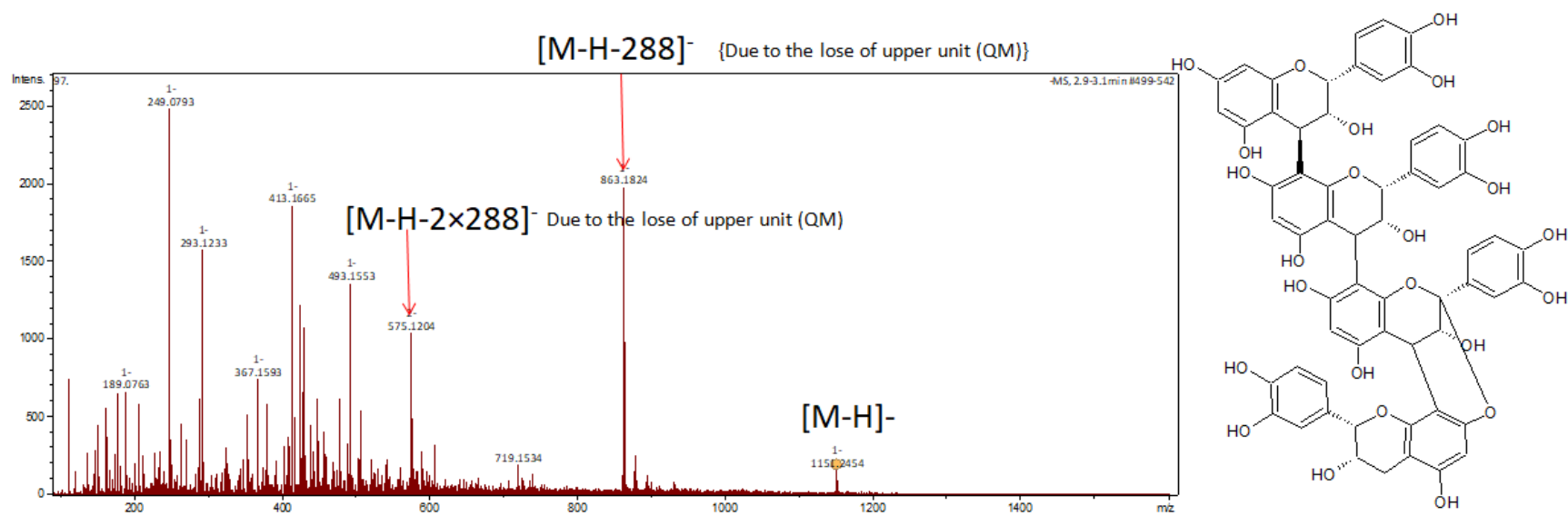


Figure S1. MS² Spectra of (epi) catechin tetramer (peak 9) [M-H]⁻ m/z 1151.2454, C₆₀H₄₈O₂₄

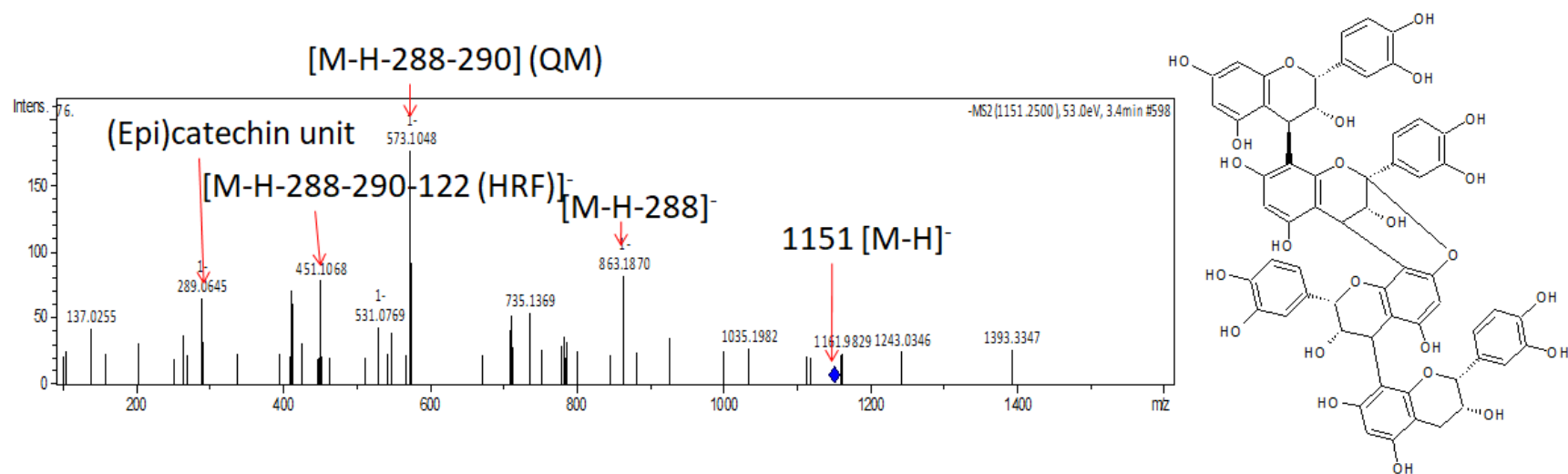


Figure S2. MS² Spectra of (epi) catechin tetramer (peak **10**) [M-H]⁻ m/z 1151.25, C₆₀H₄₈O₂₄

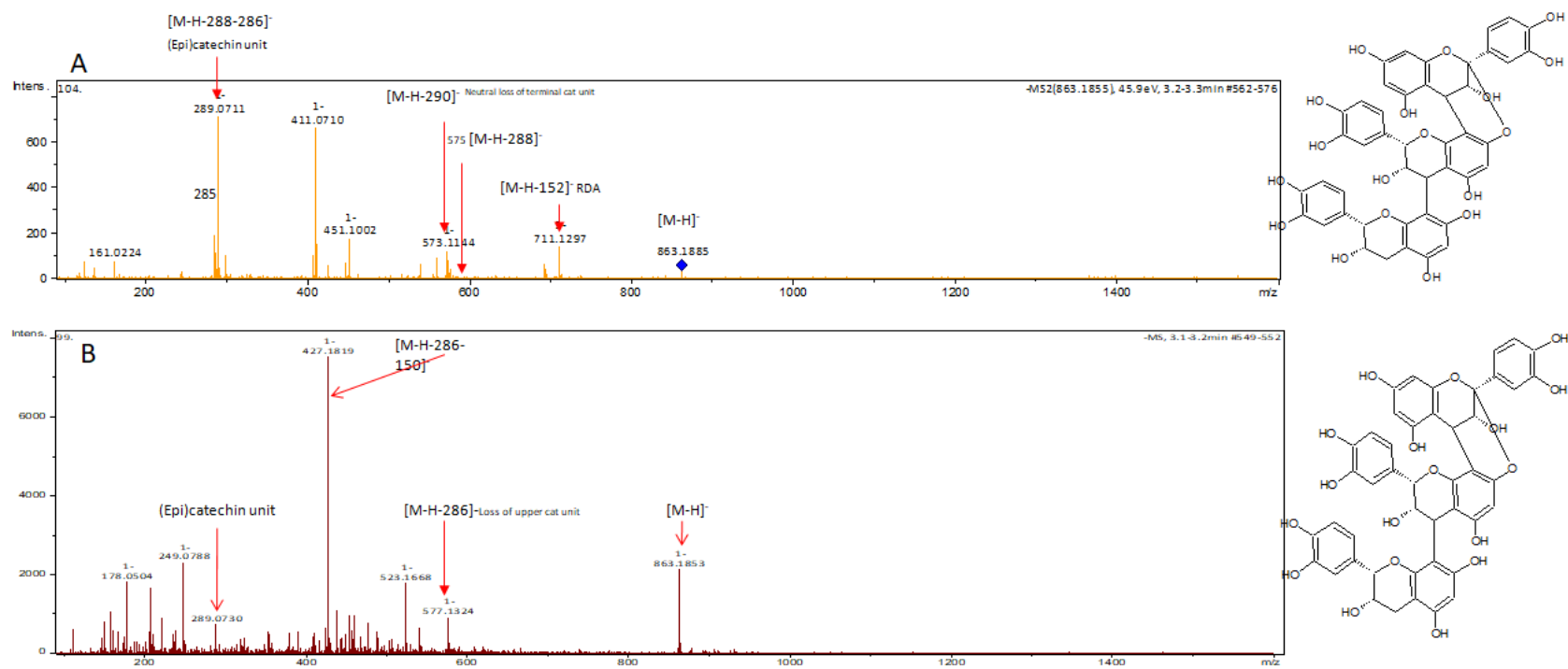


Figure S3. MS² Spectra of **A**, **B** (epi) catechin trimer A type (peaks **11**, **12**) [M-H]⁻ m/z 863.1885, C₄₅H₃₆O₁₈

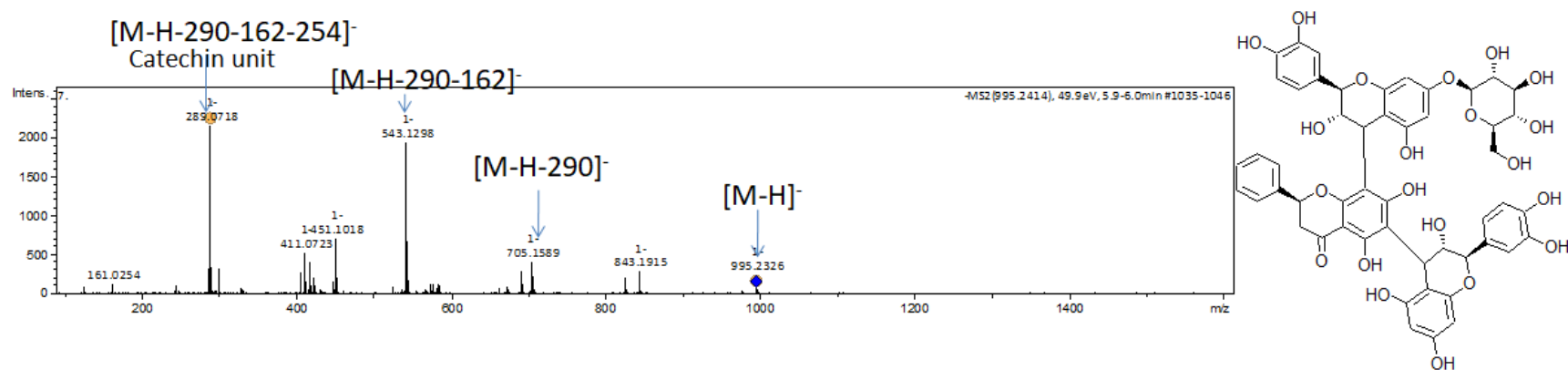


Figure S4. MS² Spectra of Catechin-chrysin-catechin-*O*-hexoside (peak **37**) [M-H]⁻ *m/z* 995.2414, C₅₁H₄₈O₂₁

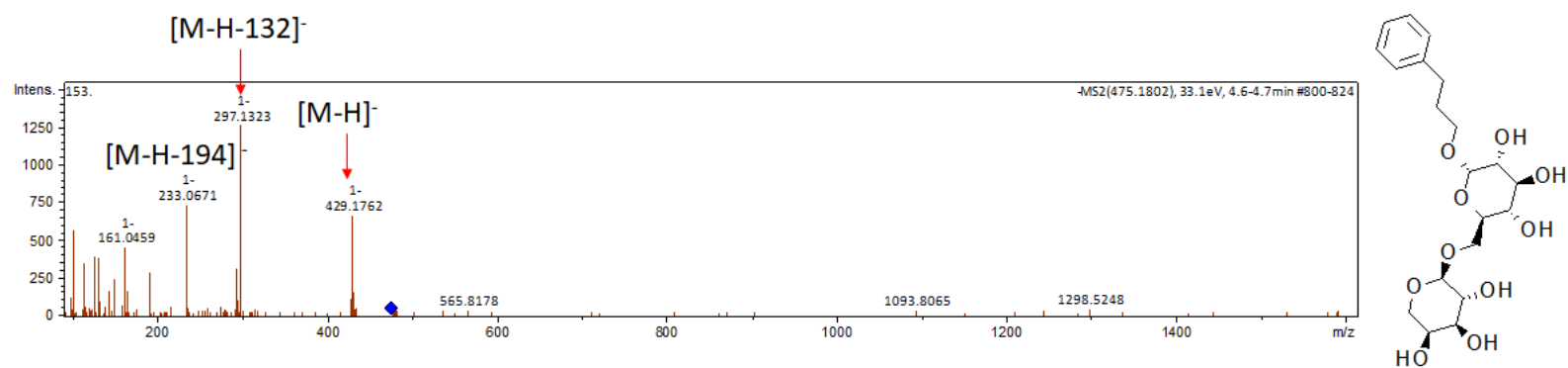


Figure S5. MS² Spectra of dihydrocinnamyl-*O*-pentosylhexoside (peak **27**) [M-H]⁻ *m/z* 429.1762, C₂₀H₃₂O₁₂

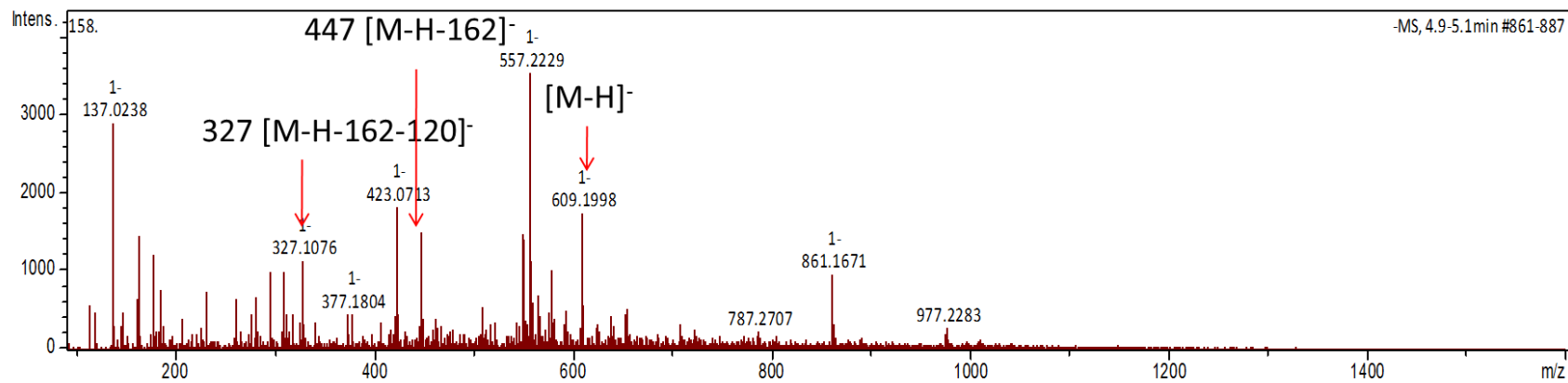


Figure S6. MS² Spectra of luteolin-*O/C*-di-hexoside (peak 30) [M-H]⁻ m/z 609.1998, C₂₇H₃₀O₁₆

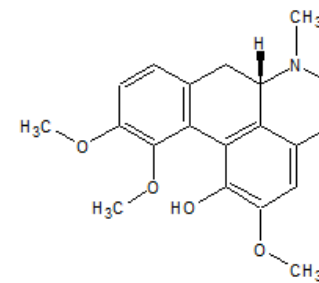
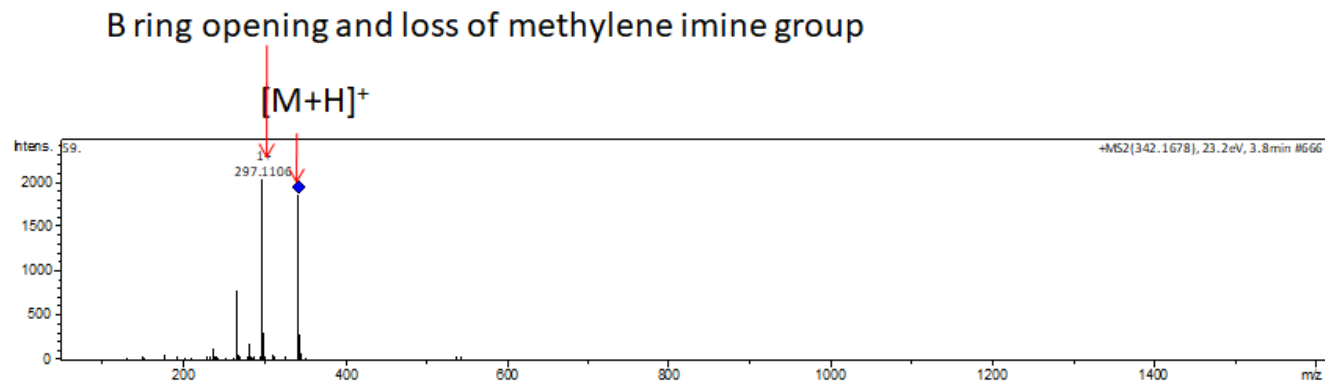


Figure S7. MS² Spectra of corydine (peak **21**) $[M+H]^+$ m/z 342.1678, C₂₀H₂₃NO₄

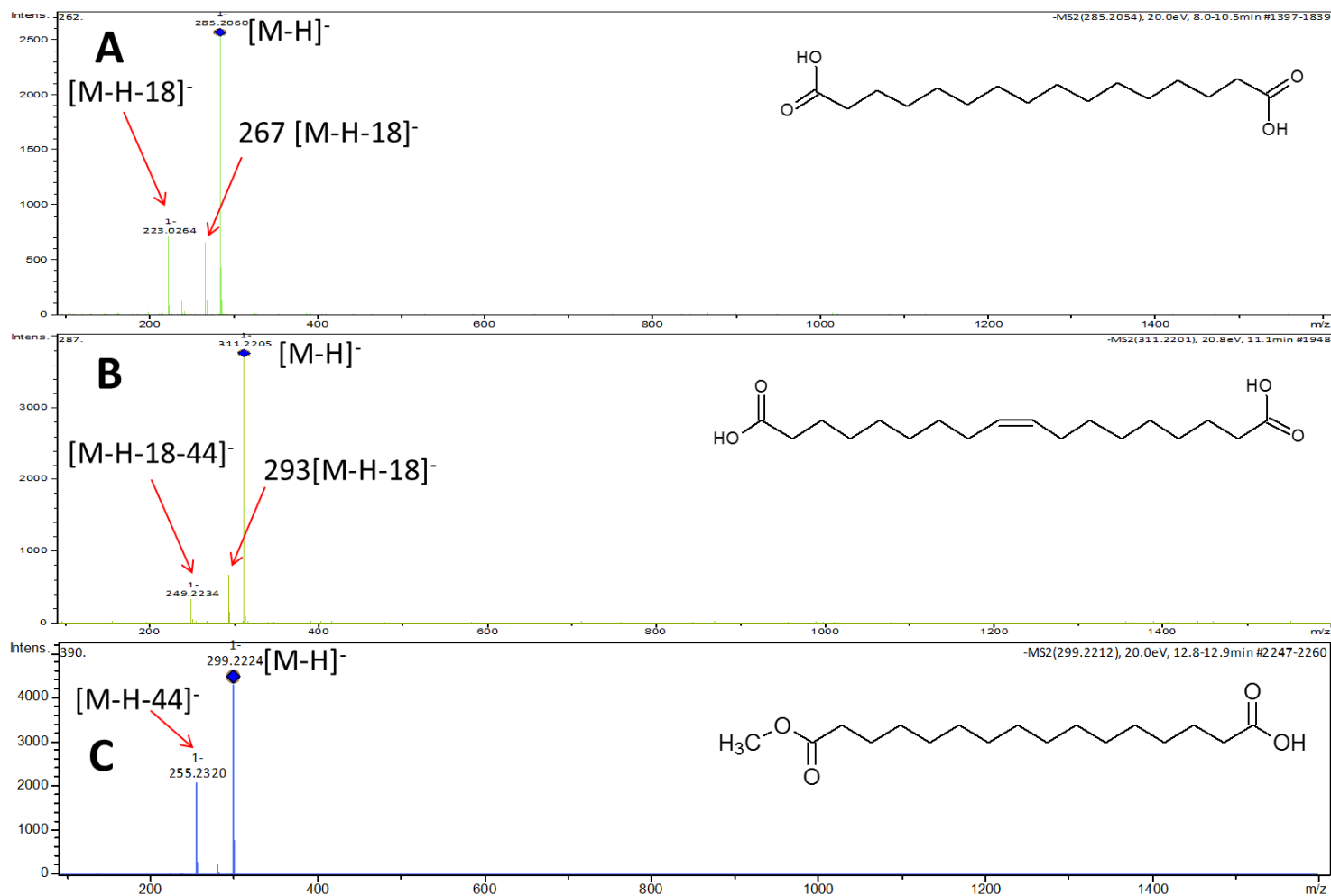


Figure S8. MS^2 Spectra of dicarboxylic fatty acids: **A** hexadecanedioic acid (peak **53**) $[M-H]^-$ m/z 285.2060, $C_{16}H_{31}O_4$; **B** octadecenedioic acid (peak **54**) $[M-H]^-$ m/z 311.2205, $C_{18}H_{32}O_4$; **C** Hexadecanedioic acid, monomethyl ester (peak **57**) $[M-H]^-$ m/z 299.2060, $C_{17}H_{32}O_4$

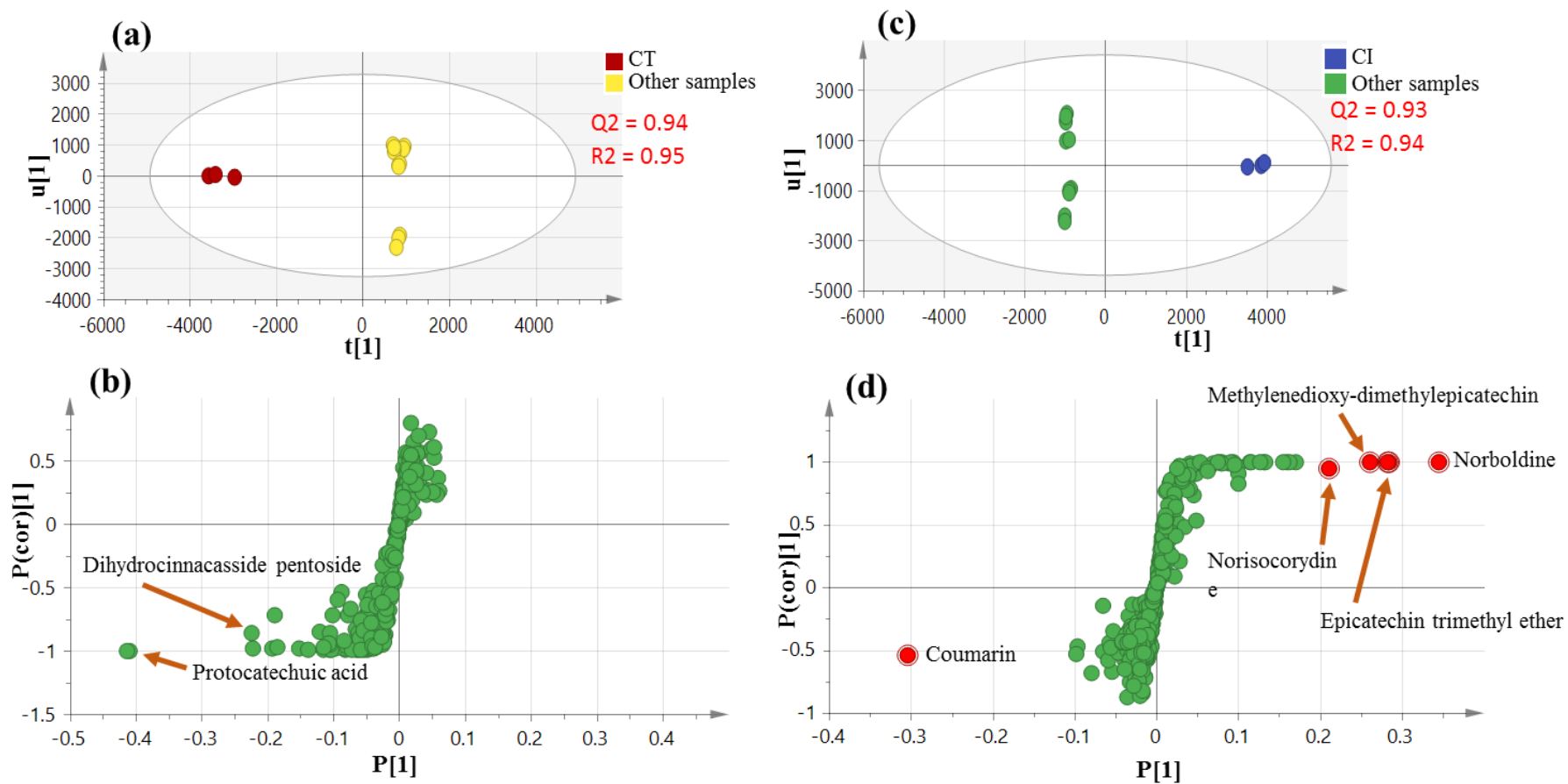


Figure S9. UPLC-MS OPLS-DA (a) score plot and (b) loading S-plots derived from modelling CT (*C. tamala* from Pakistan) against other samples in a separate group on negative ion mode. OPLS-DA (c) score plot and (d) loading S-plots derived from modelling CI (*C. iners* from Malaysia) against other samples in a separate group on positive ion mode.

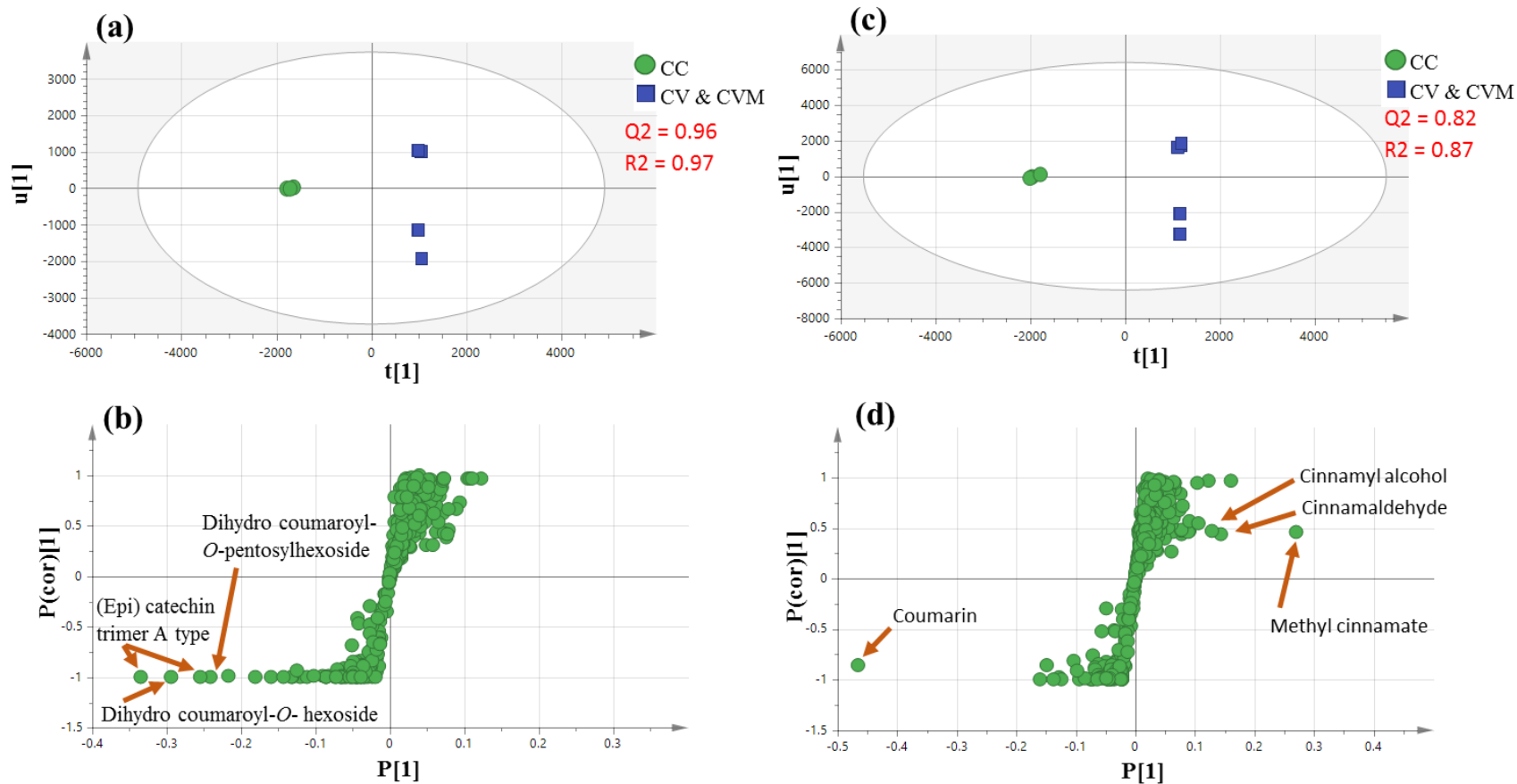


Figure S10. UPLC-MS OPLS-DA (a) score plot and (b) loading S-plots derived from modelling CC (*Cinnamomum cassia* from Malaysia) versus CV (*C. verum* from Pakistan) and CVM (*C. verum* from Malaysia) in a separate group on negative ion mode. OPLS-DA (c) score plot and (d) loading S-plots derived from modelling CC versus CV and CVM on positive ion mode. Each S-plot revealed the covariance $p[1]$ against the correlation $p(\text{cor})[1]$ of the variables of the discriminating component.

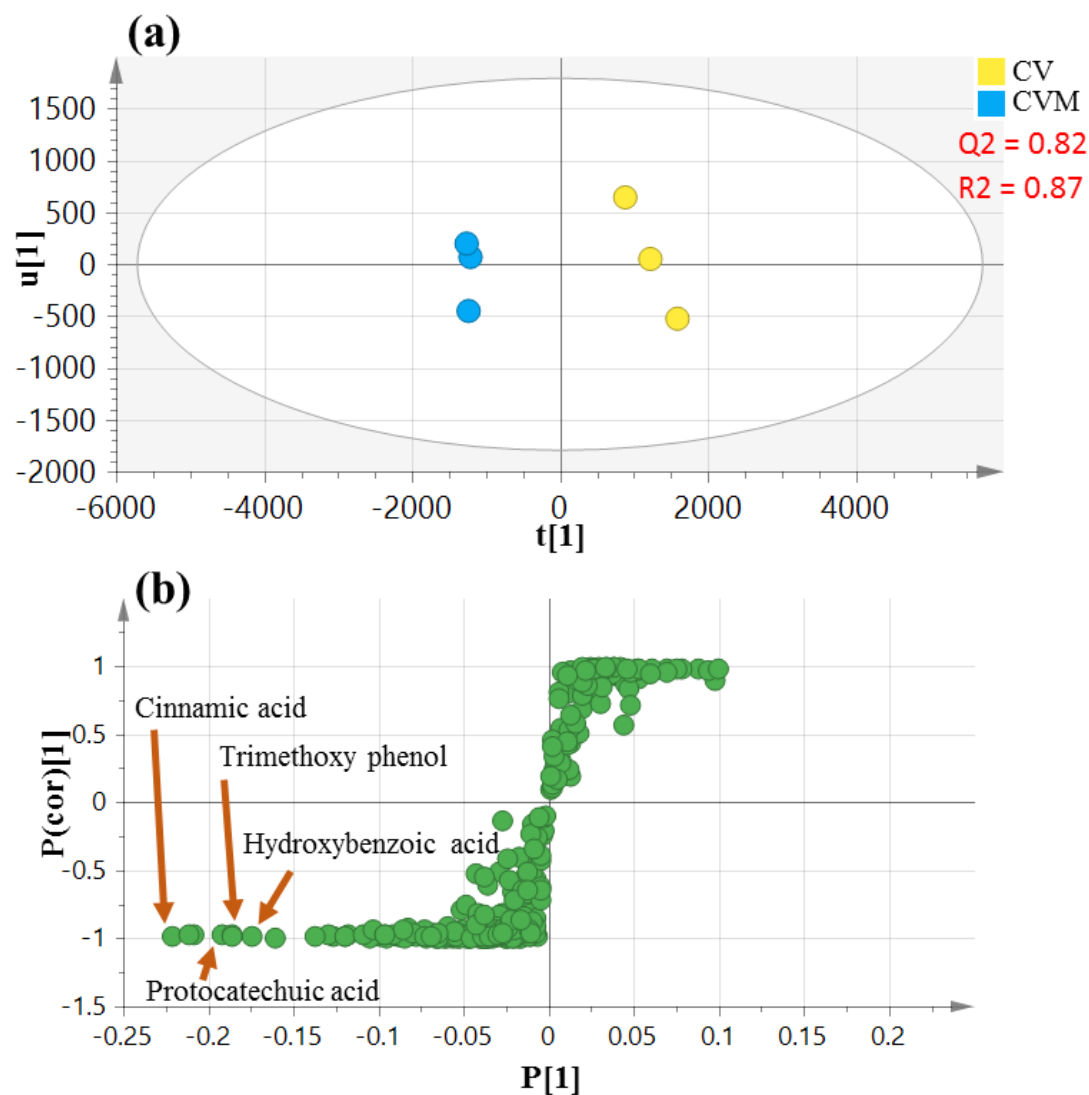


Figure S11. UPLC-MS OPLS-DA (a) score plot and (b) loading S-plots derived from modelling CV (*C. verum* from Pakistan) versus CVM (*C. verum* from Malaysia) on negative ion mode revealing the covariance $p[1]$ against the correlation $p(\text{cor})[1]$ of the variables of the discriminating component.

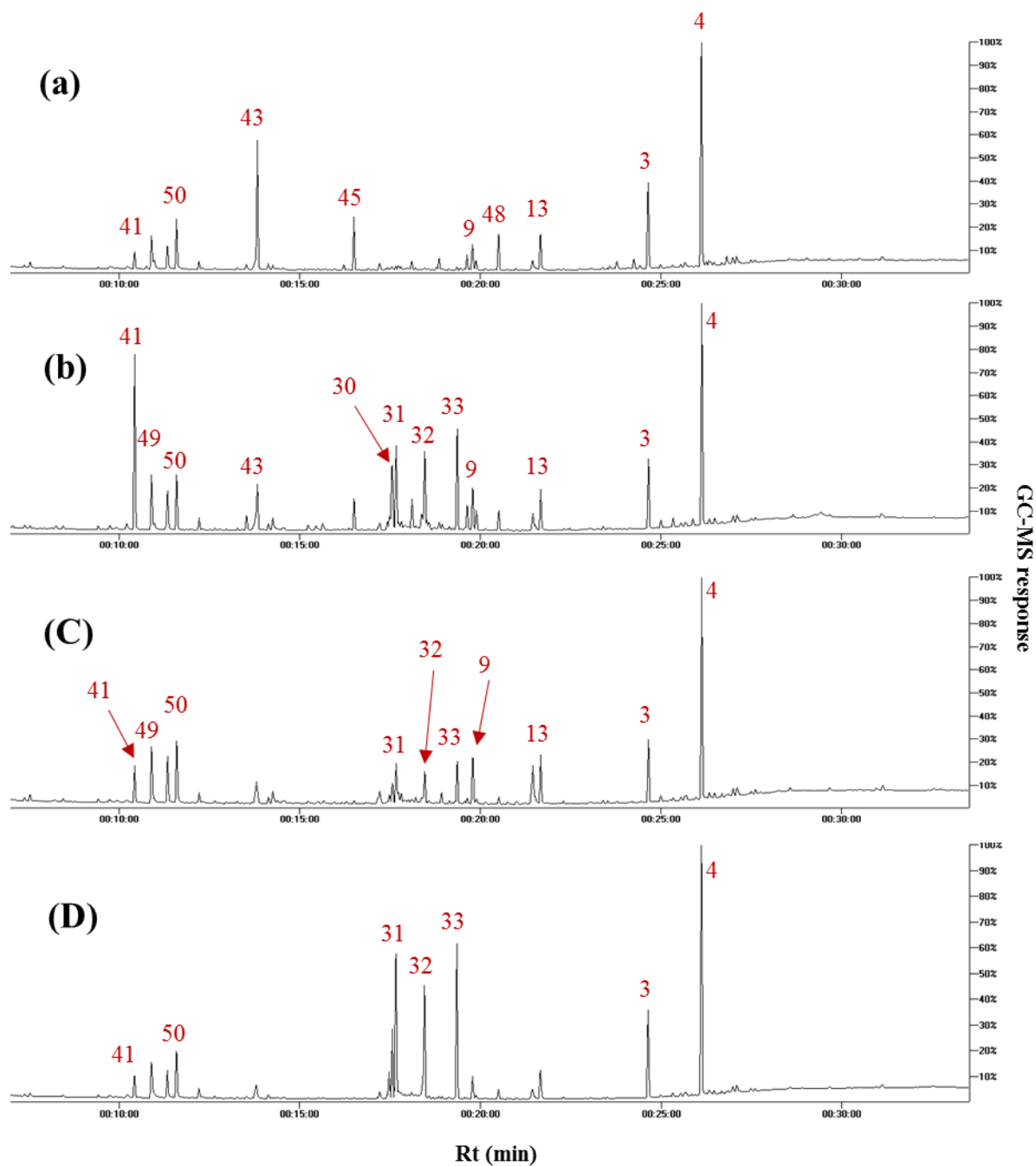


Figure S12. Representative SPME-GC-MS chromatograms of cinnamon primary metabolites, acquired from (a) CI (*C. iners* from Malaysia), (b) CT (*C. tamala* from Pakistan) and (c) CV (*C. verum* from Pakistan).

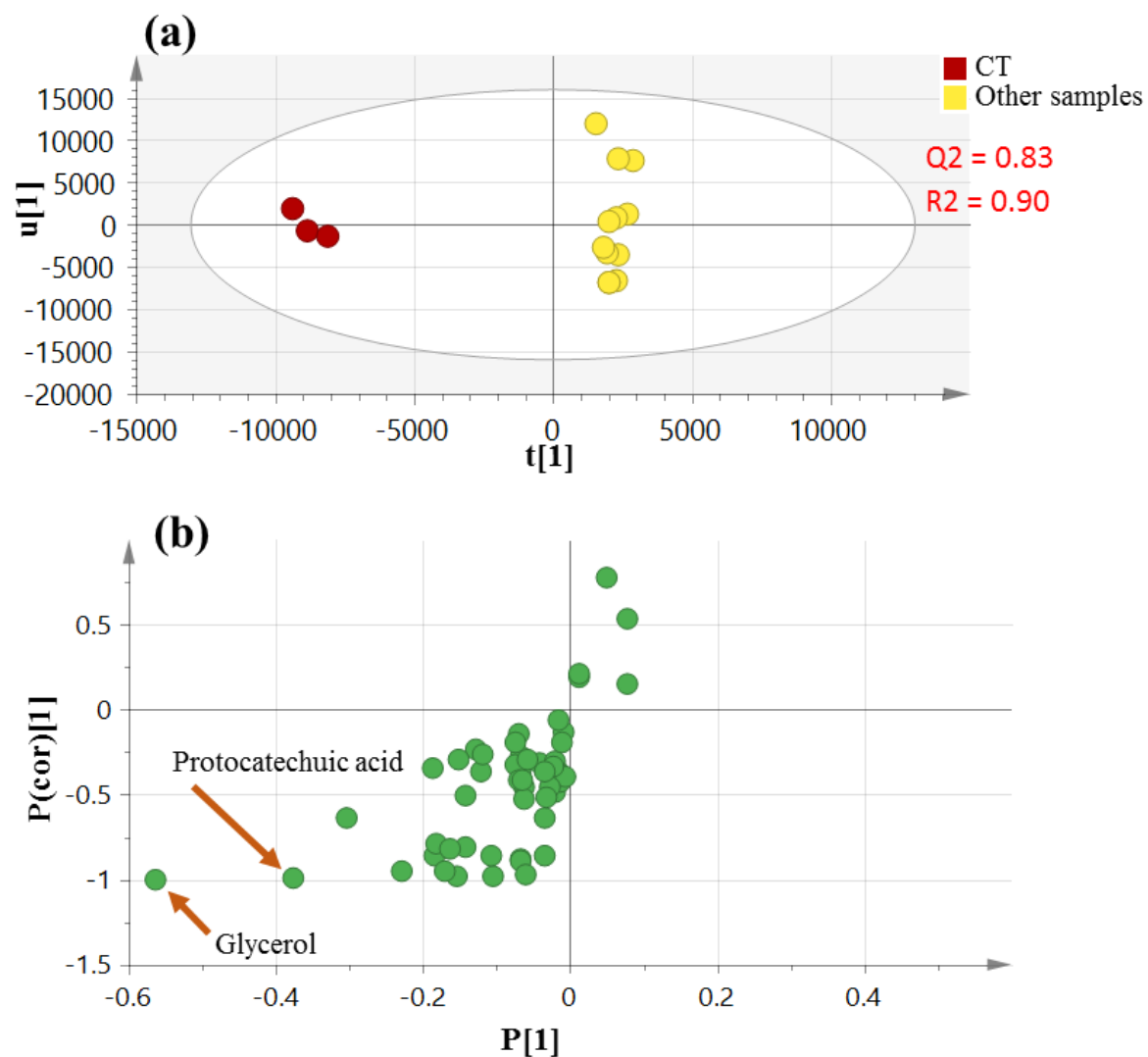


Figure S13. GC-MS OPLS-DA (a) score plot and (b) loading S-plots derived from modelling CT (*C. tamala* from Pakistan) versus all other samples revealing the covariance $p[1]$ against the correlation $p(\text{cor})[1]$ of the variables of the discriminating component.

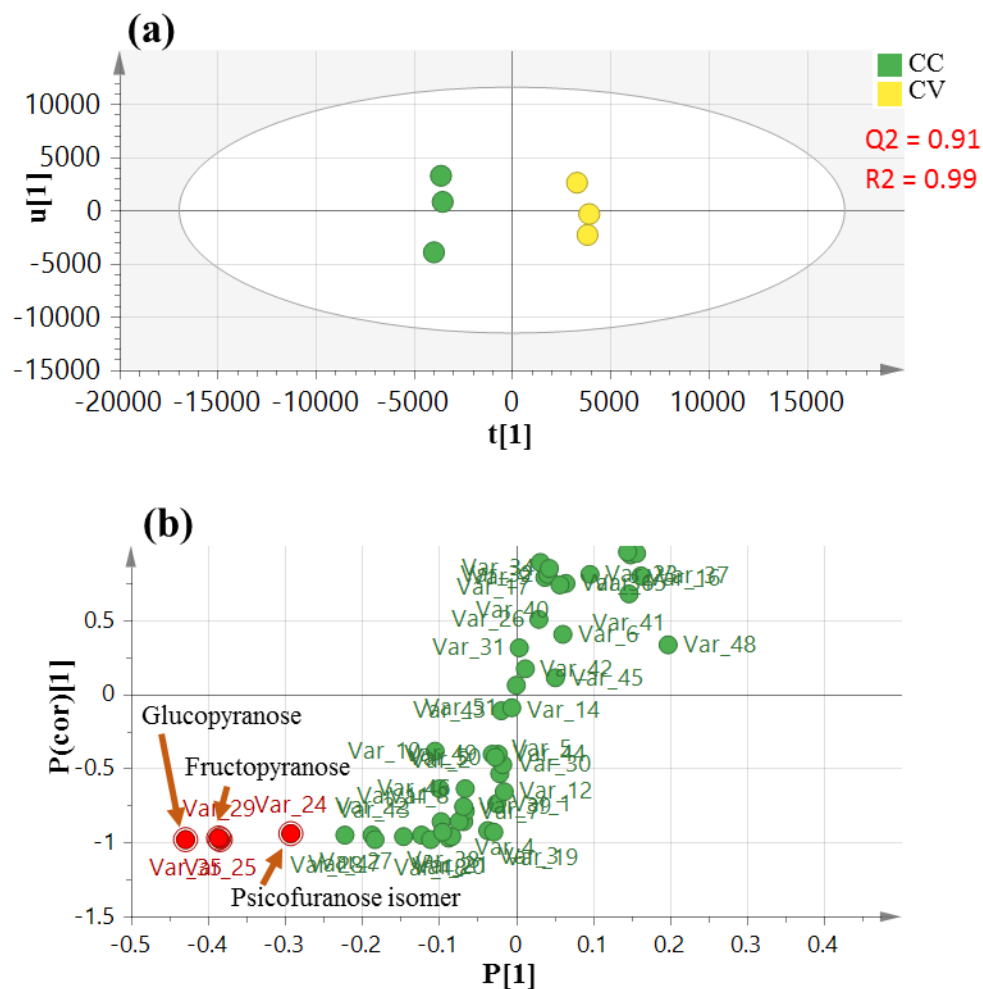


Figure S14. GC-MS OPLS-DA (a) score plot and (b) loading S-plots derived from modelling CC (*Cinnamomum cassia* from Malaysia) versus CV (*C. verum* from Pakistan) revealing the covariance $p[1]$ against the correlation $p(\text{cor})[1]$ of the variables of the discriminating component.