Supplementary information

Effect-directed profiling of strawberry varieties and breeding materials via planar chromatography and chemometrics

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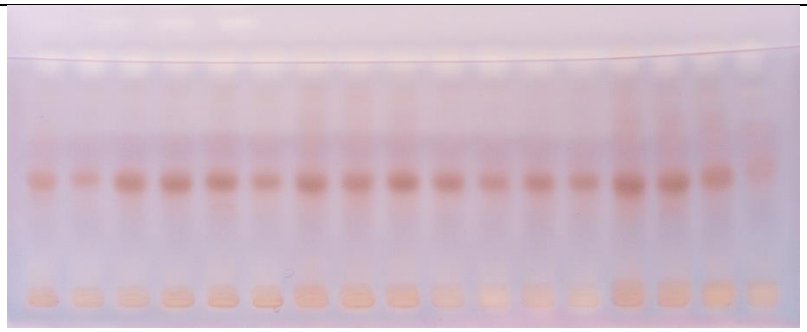
Content

Table S1. Bond dissociation enthalpy (BDE) and ionization potential (IP) given in kJ/mol calculated for pelargonidin-3-*O*-glucoside monoanion at M062X/6-31+g(d,p) level in the gas phase, and using SMD solvation models of water and pentyl ethanoate.

Protonation state	Site	Gas phase		Water		Pentyl ethanoate	
		BDE	IP	BDE	IP	BDE	IP
5–*O* anion	4′-OH	371	674	382	456	371	505
	7-OH	357		383		363	

a) *Bacillus subtillis* bioassay

b) Butyrylcholinesterase inhibition assay



c) Acetylcholinesterase inhibition assay

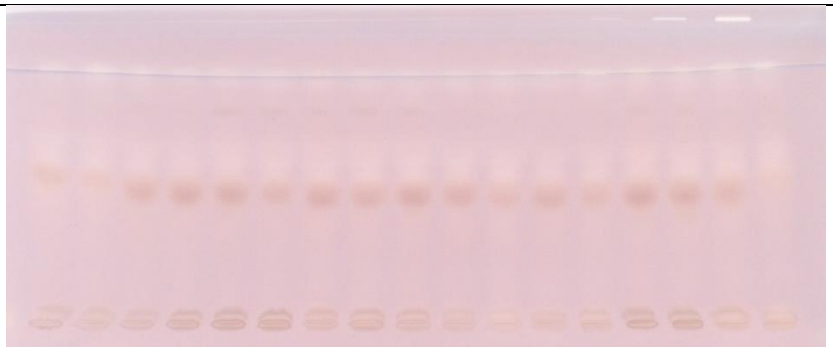


Figure S1. HPTLC profiles of 17 samples of six strawberry cultivars after (a) *Bacillus subtillis* bioassay, (b) acetylcholinesterase and (c) butyrylcholinesterase inhibition assays; respective positive controls of each assay are evident at the upper plate part

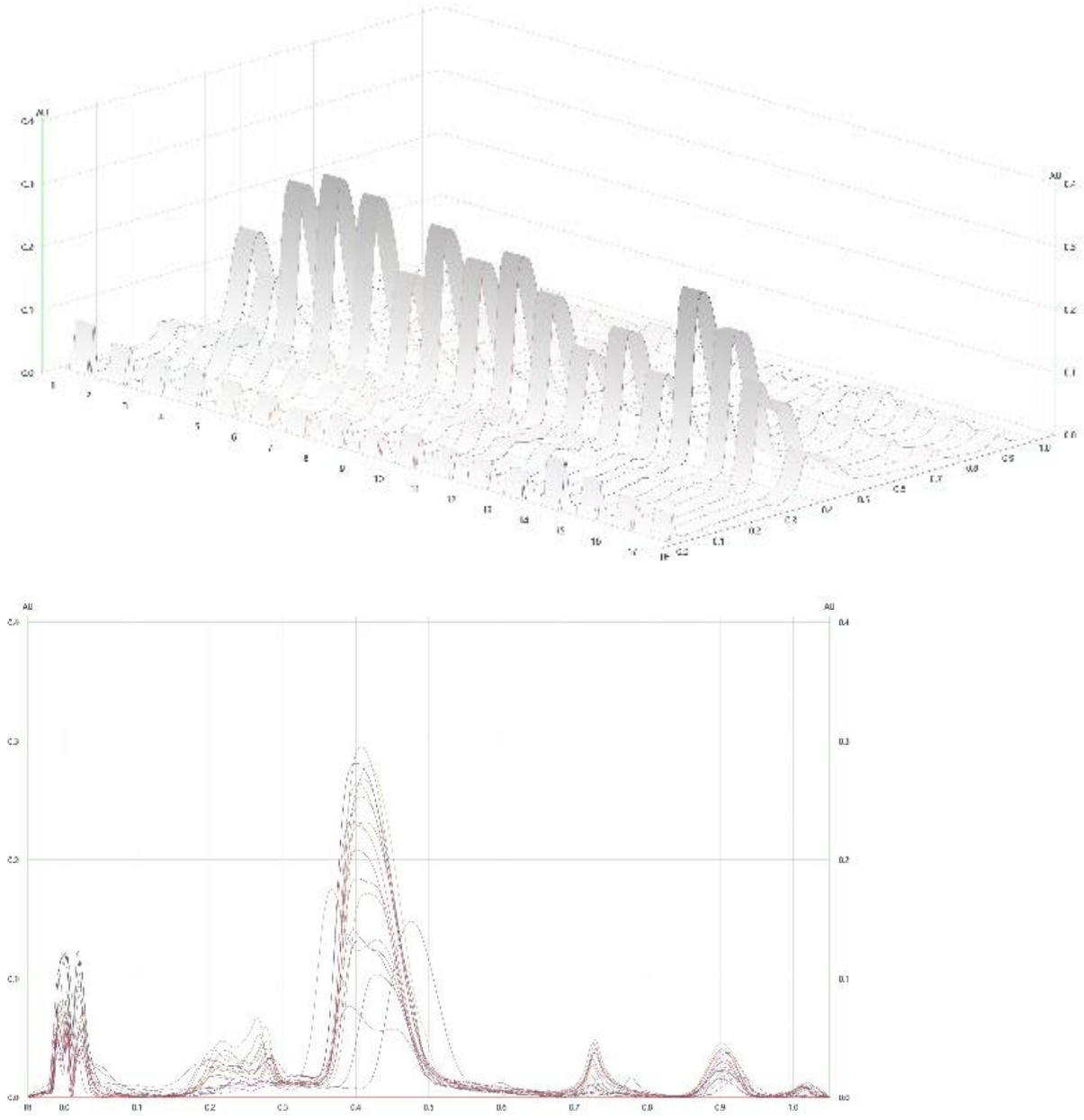
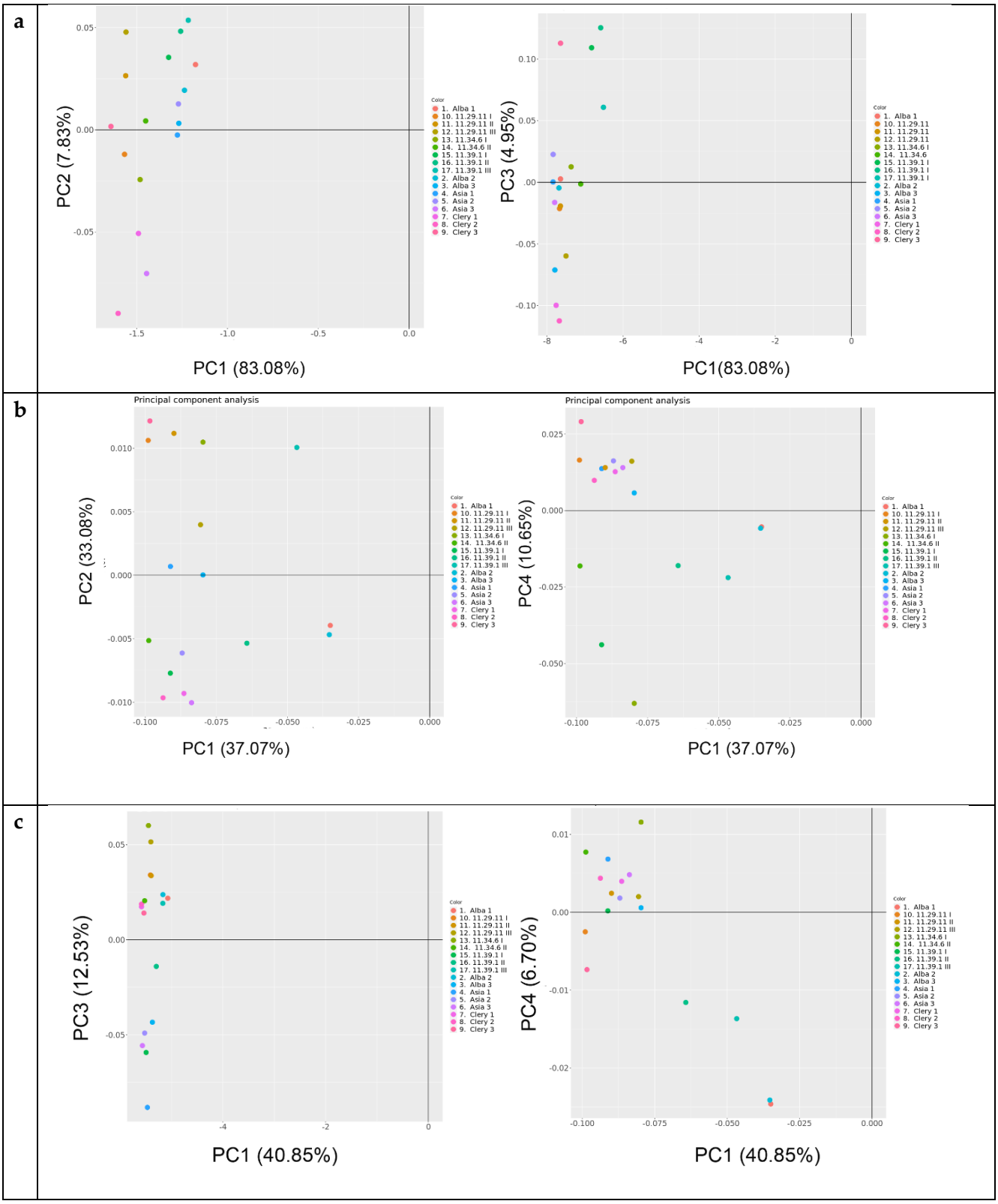


Figure S2. HPTLC densitogram of the absorbance measurement at 500 nm of 17 samples of six strawberry cultivars


a
PC2 (7.83%)
PC1 (83.08%)
PC3 (4.95%)
PC1(83.08%)
b
Principal component analysis
PC2 (33.08%)
PC1 (37.07%)
Principal component analysis
PC4 (10.65%)
PC1 (37.07%)
c
PC3 (12.53%)
PC1 (40.85%)
PC4 (6.70%)
PC1 (40.85%)
Color
1. Alba 1
10. 11.29.11 I
11. 11.29.11 II
12. 11.29.11 III
13. 11.34.6 I
14. 11.34.6 II
15. 11.39.1 I
16. 11.39.1 II
17. 11.39.1 III
2. Alba 2
3. Alba 3
4. Asia 1
5. Asia 2
6. Asia 3
7. Clery 1
8. Clery 2
9. Clery 3

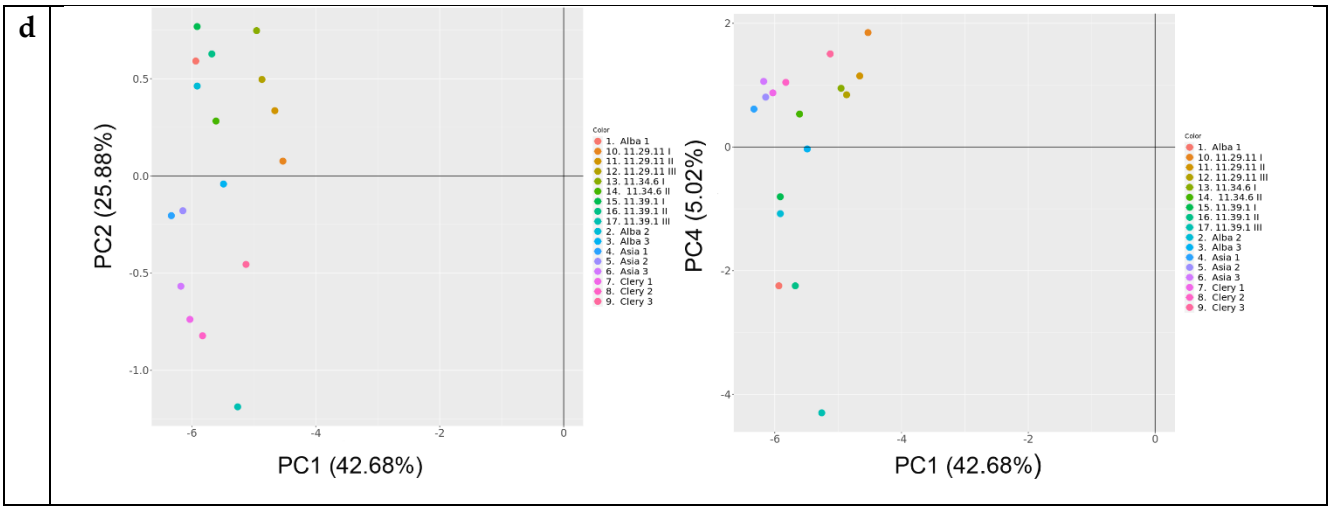


Figure S3. PCs score plots based on chromatogram at white light illumination (a), chromatogram at 254 nm absorbance (b), DPPH• scavenging autogram (c), and *Aliivibrio fischeri* bioautogram (d)