# SUPPLEMENTARY MATERIAL

## INDEX

**PHENOLIC COMPOUNDS CHROMATOGRAMS**

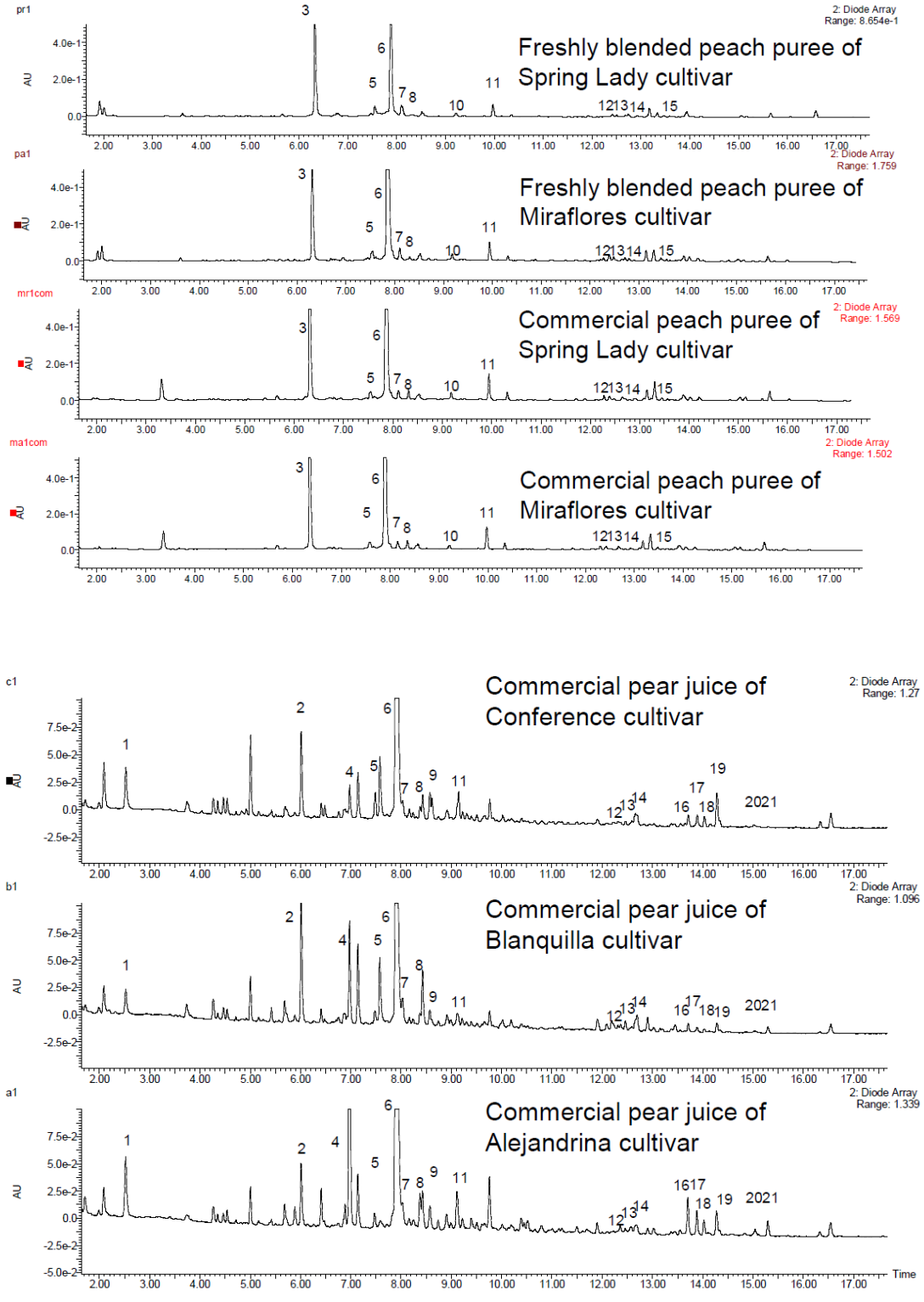



Figure 1. Chromatograms at 350 + 280 + 320 nm of pear juices and peach purees. Numbered according the next table.

| Peak number | Compound | UV max (nm) |
|---|---|---|
| 1 | Hydroquinone β-D-glucopyranoside or Arbutin [a] (Arb) | 283 |
| 2 | Protocatechuic aldehyde monoglucuronide [b] (ProCat-glu) | 268 |
| 3 | 3-Caffeoylquinic acid [b] (3-Caf-qui) | 240, 326 |
| 4 | Coumaroyl-hexose [b] (Cou-hex) | 316 |
| 5 | Procyanidin-B1 [a] (Pro-B1) | 278 |
| 6 | 5-Caffeoylquinic acid [a] (5-Caf-qui) | 240, 326 |
| 7 | (+)-Catechin [a] (Cat) | 278 |
| 8 | 4-Caffeoylquinic acid [b] (4-Caf-qui) | 240, 326 |
| 9 | Procyanidin-B2 [a] (Pro-B2) | 278 |
| 10 | 5-*p*-Coumaroylquinic acid [b] (5-p-Cou-qui) | 235, 312 |
| 11 | (-)-Epicatechin [a] (Epi) | 278 |
| 12 | Quercetin-3-*O*-rutinoside [a] (Q-rut) | 255, 353 |
| 13 | Quercetin-3-*O*-galactoside [a] (Q-gal) | 255, 353 |
| 14 | Quercetin-3-*O*-glucoside [a] (Q-glu) | 255, 353 |
| 15 | Kaempferol 3-*O*-rutinoside [a] (K-rut) | 265, 347 |
| 16 | Isorhamnetin-3-*O*-robinioside [b] (Iso-rob) | 254, 352 |
| 17 | Isorhamnetin-3-*O*-rutinoside [a] (Iso-rut) | 254, 352 |
| 18 | Isorhamnetin-3-*O*-galactoside [b] (Iso-gal) | 254, 352 |
| 19 | Isorhamnetin-3-*O*-glucoside [b] (Iso-glu) | 254, 352 |
| 20 | Isorhamnetin 3-*O*-malonygalactoside [b] (Iso-malgal) | 254, 352 |
| 21 | Isorhamnetin 3-*O*-6″-malonygalactoside [b] (Iso-6″-malgal) | 254, 352 |

## ION SPECTRA FROM CAFFEOYLQUINIC ACID ISOMERS

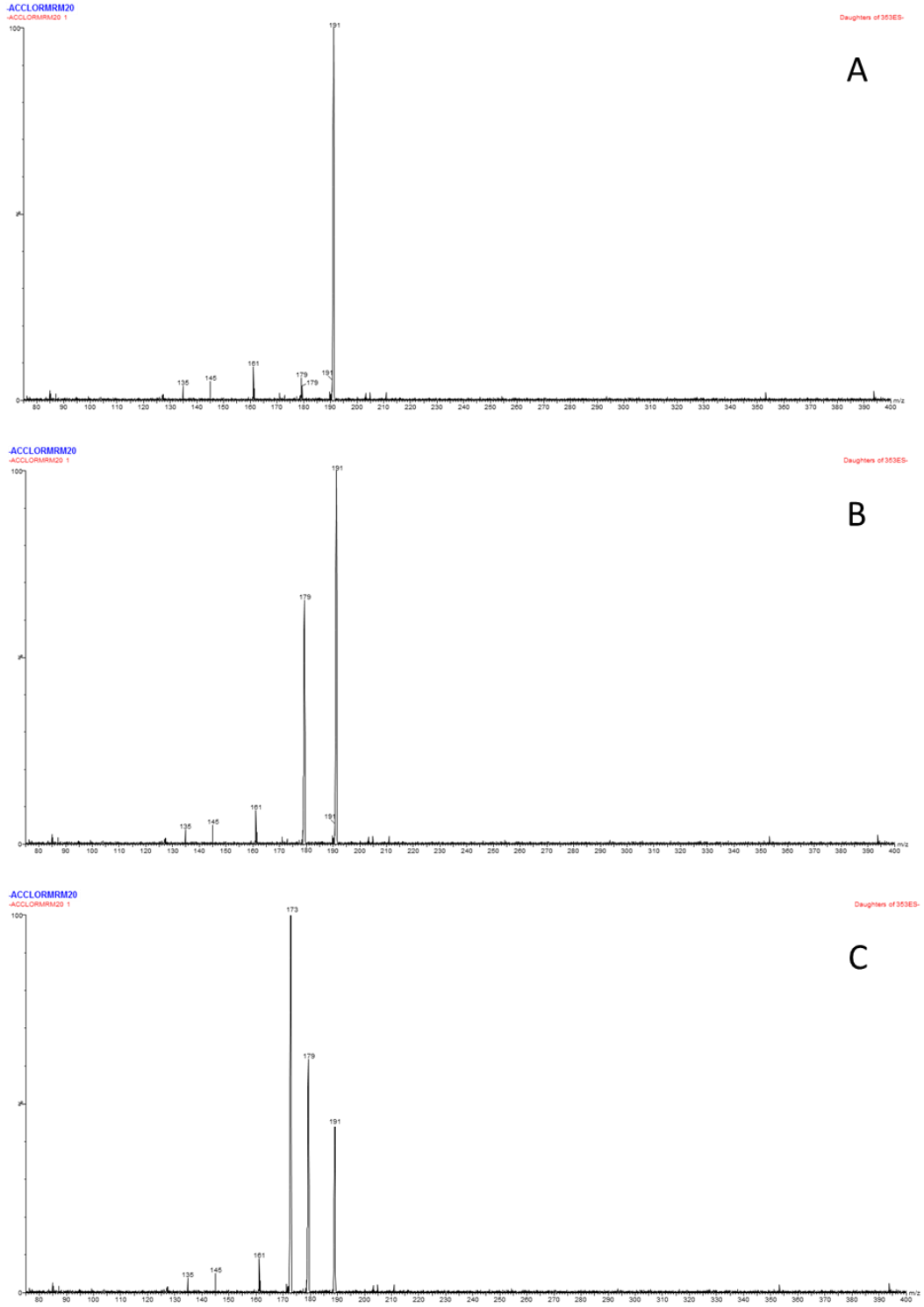
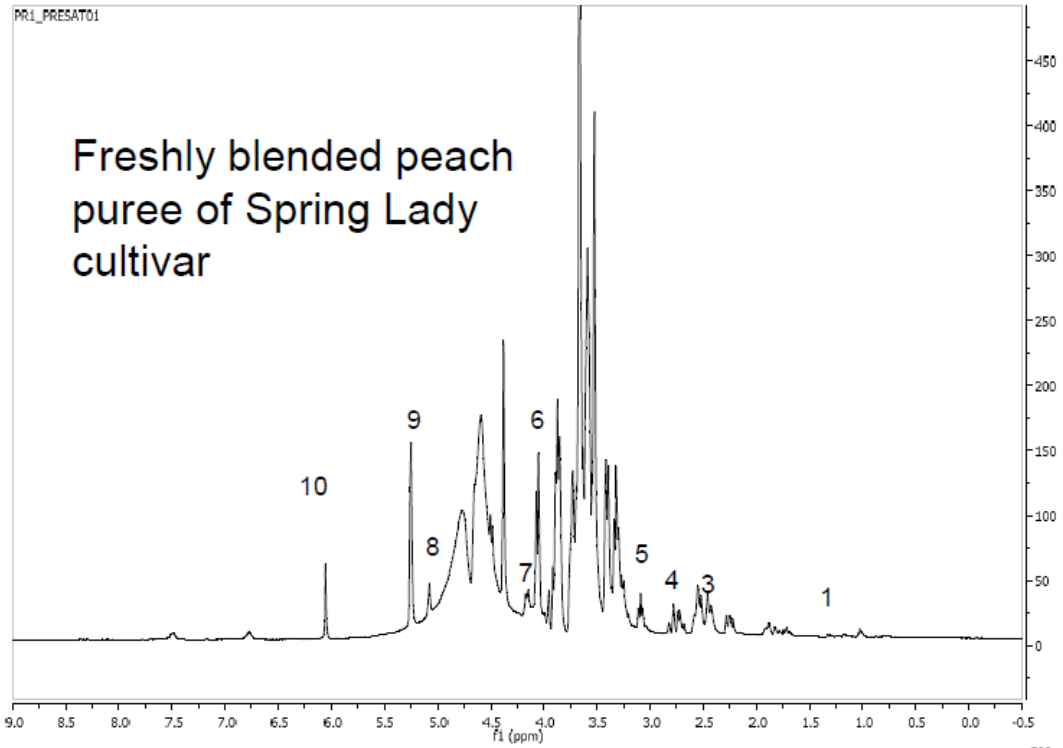
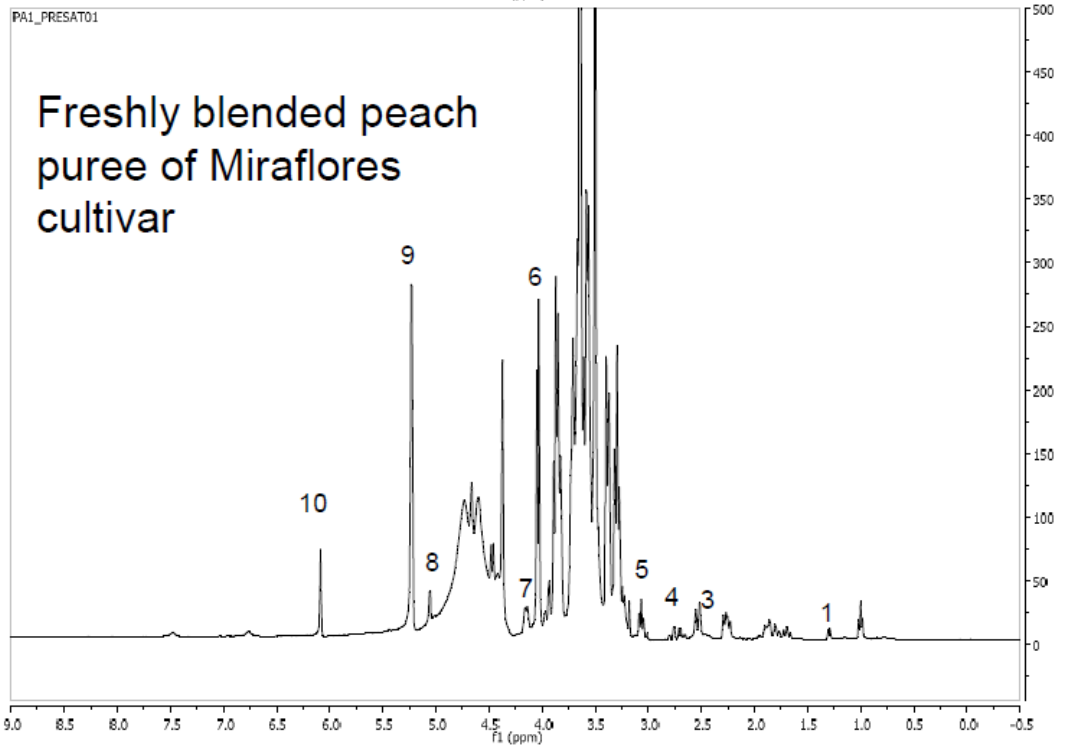
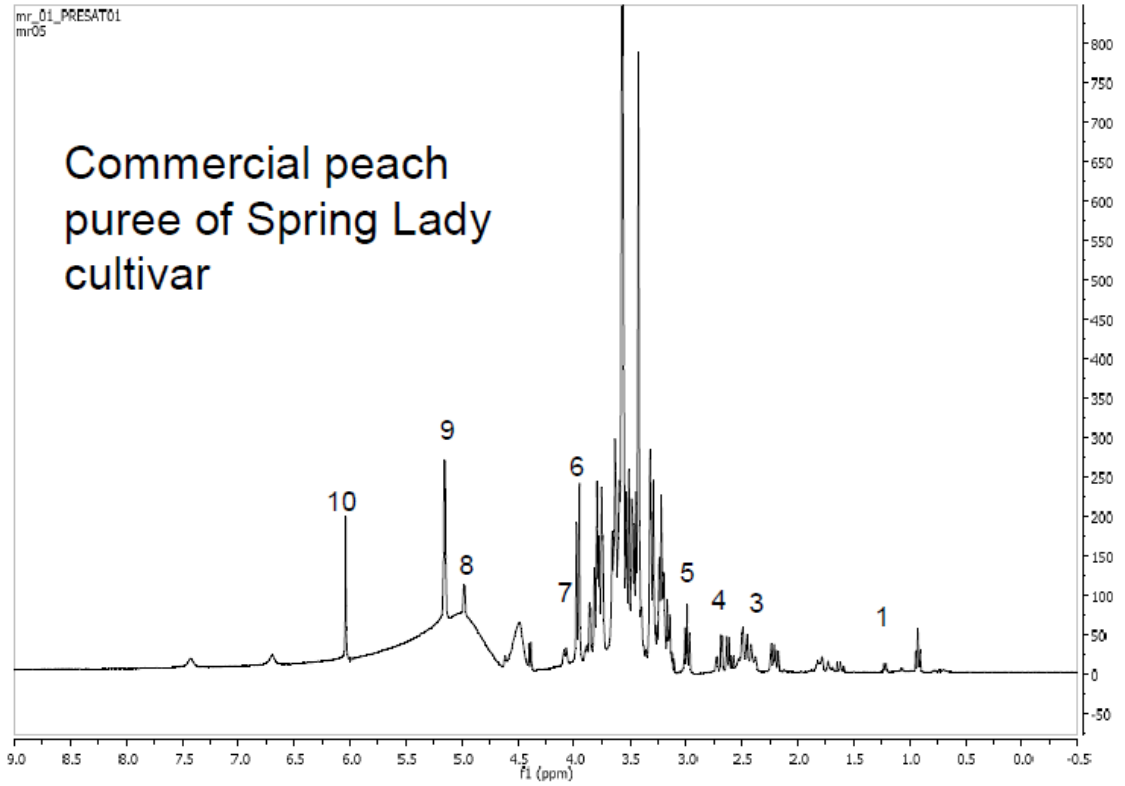


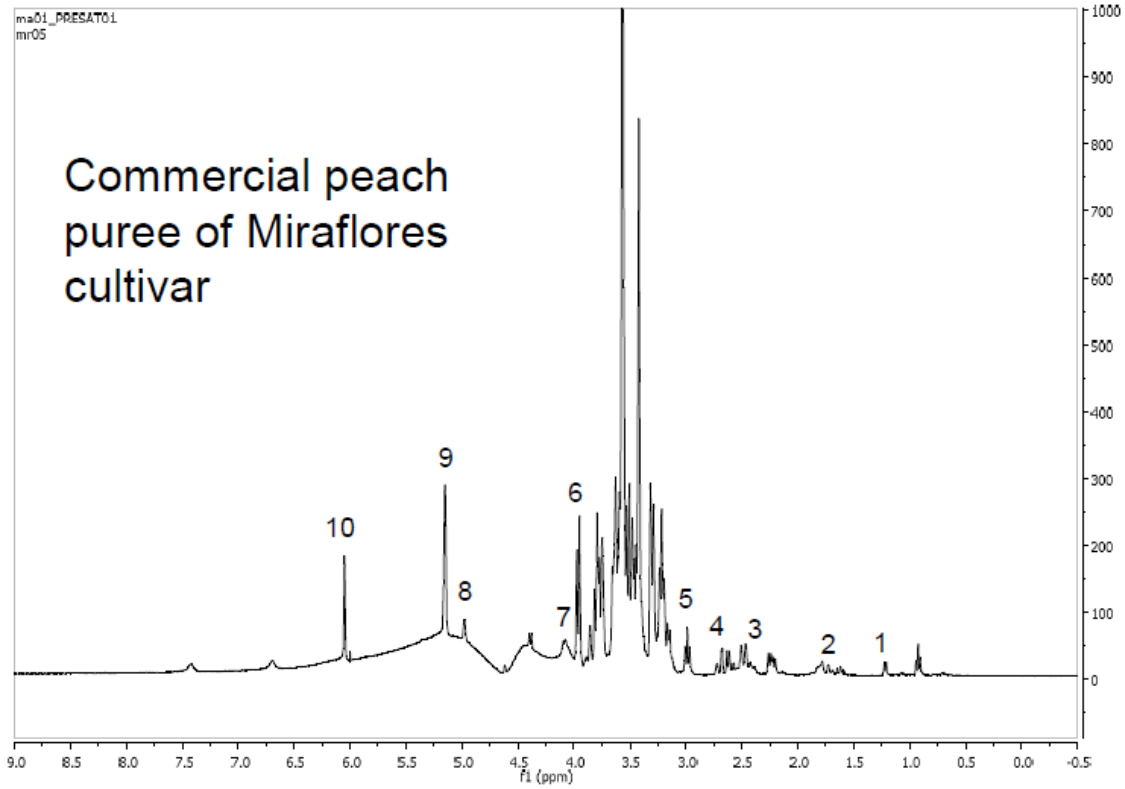

Figure 2. Ion spectra of caffeoylquinic isomers: **A**: 5-Caffeoylquinic acid (5-Caf-qui), **B**: 3-Caffeoylquinic acid (3-Caf-qui) and **C**: 4-Caffeoylquinic acid (4-Caf-qui).

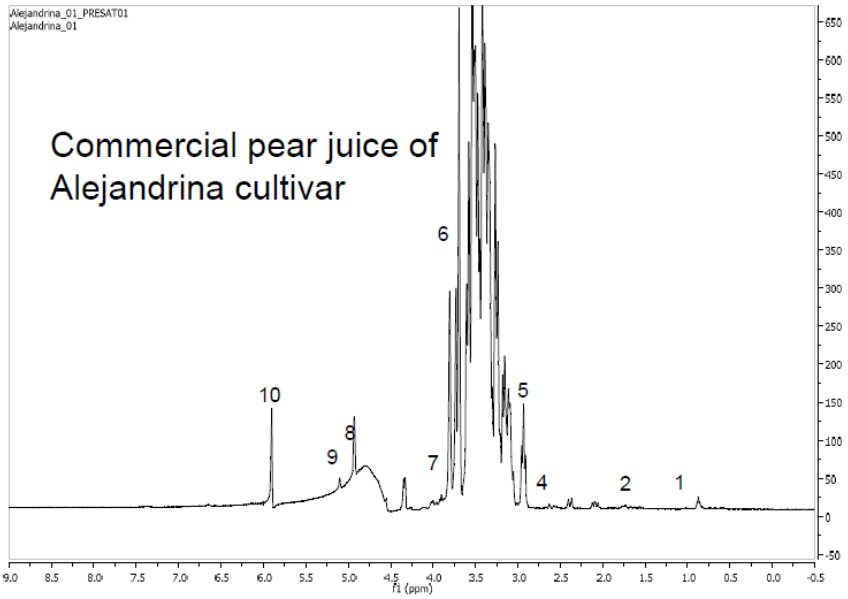
## $^{1}$H NMR SPECTRA

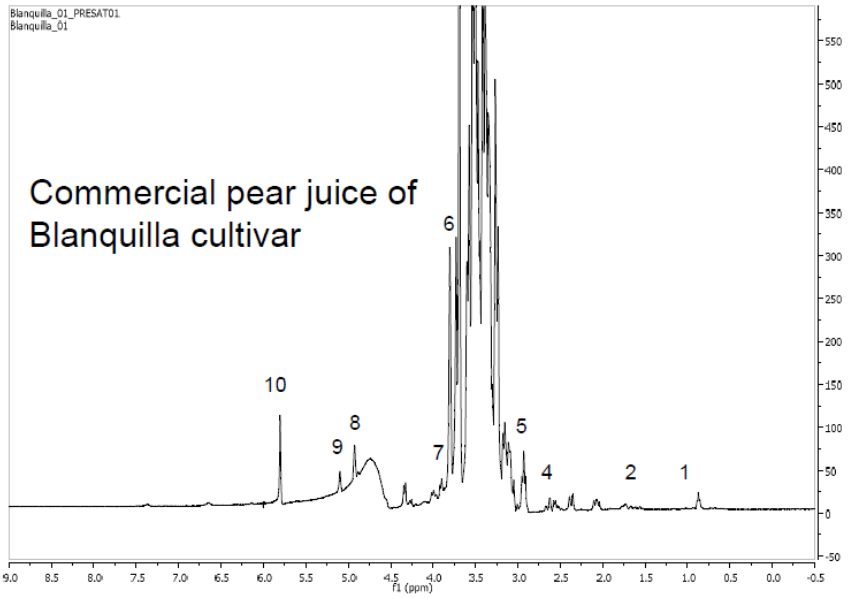



mr_01_PRESAT01
mr05
Commercial peach puree of Spring Lady cultivar
10
9
8
7
6
5
4
3
1
f1 (ppm)


ma01_PRESAT01
mr05
Commercial peach puree of Miraflores cultivar
10
9
8
7
6
5
4
3
2
1
f1 (ppm)


Alejandrina_01_PRESAT01
Alejandrina_01
Commercial pear juice of
Alejandrina cultivar
10
9
8
7
6
5
4
2
1
F1 (ppm)


Blanquilla_01_PRESAT01
Blanquilla_01
Commercial pear juice of
Blanquilla cultivar
10
9
8
7
6
5
4
2
1
F1 (ppm)

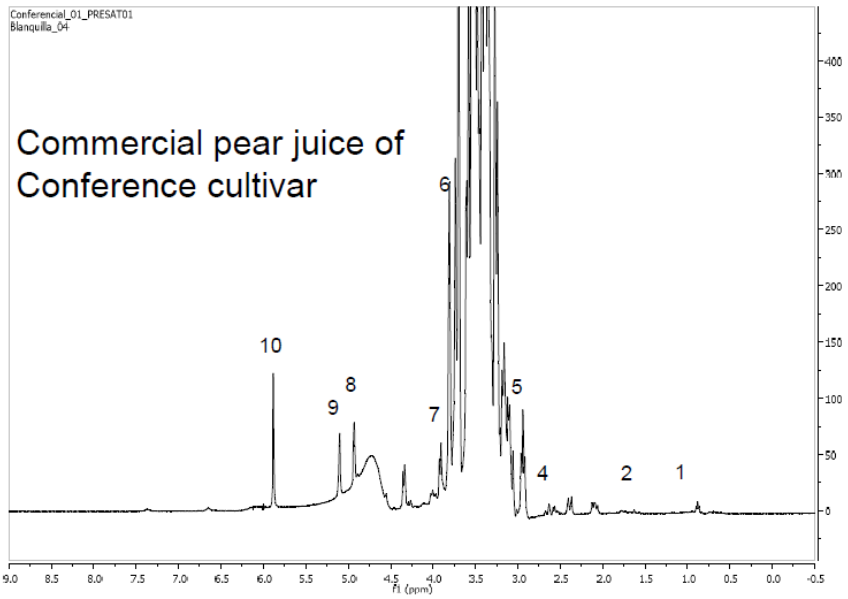

Conferencial_01_PRESAT01
Blanquilla_04
Commercial pear juice of
Conference cultivar
10
9
8
7
6
5
4
2
1
F1 (ppm)

Figure 3. $^{1}$H NMR spectra of commercial pear juices and peach purees. Numbered according the next table.

| Signal number | Compound | Assignment | $^{1}$H (ppm) |
|---|---|---|---|
| 1 | Alanine (ALA) | β-$CH_3$ | 1.49 |
| 2 | Quinic acid (QA) | $CH_2$-1,1′; $CH_2$-5,5′ | 1.7 |
| 3 | Citric acid (CA) | α,γ-CH | 2.3 |
| 4 | Asparagine (ASP) | β, β′-$CH_2$ | 2.7 |
| 5 | β-Glucose (βGLC) | CH-2 | 2.95 |
| 6 | β-D-Fructopyranose(FRU) | $CH_2$-6,6′ | 3.85 |
| 7 | Malic acid (MA) | β, β′-$CH_2$ | 4.1 |
| 8 | α-Glucose (αGLC) | CH-1 | 4.95 |
| 9 | Sucrose (SUCR) | GLC CH-1 | 5.15 |
| 10 | Maleic acid (IS) | 2CH | 5.9 |

## ANOVA RESULTS

**Peach puree samples**

Oneway Anova p-value cut-off:.0.05

| Compound | p | FC ([PM] vs [PSL]) | FC ([PM] vs [UnPM]) | FC ([PM] vs [UnPSL]) | FC ([PSL] vs [UnPM]) | FC ([PSL] vs [UnPSL]) | FC ([UnPM] vs [UnPSL]) |
|---|---|---|---|---|---|---|---|
| **SUCR** | 1.42E−04 | 1.48 | −1.02 | 1.43 | −1.51 | −1.03 | 1.46 |
| **FRU** | 4.94E−02 | −1.12 | −1.24 | −1.22 | −1.11 | −1.08 | 1.02 |
| **bGLUC** | 2.06E−02 | −1.08 | −1.05 | −1.25 | 1.03 | −1.15 | −1.19 |
| **ASP** | 3.42E−05 | −1.42 | 1.45 | −1.22 | 2.05 | 1.16 | −1.77 |
| **CA** | 1.06E−06 | −1.95 | 1.14 | −2.27 | 2.22 | −1.17 | −2.59 |
| **MA** | 4.35E−03 | 1.15 | −1.23 | −1.11 | −1.42 | −1.28 | 1.11 |
| **QA** | 1.46E−02 | 1.33 | 1.14 | 1.45 | −1.17 | 1.09 | 1.27 |
| **3-Caf-qui** | 1.15E−02 | 1.46 | 1.23 | 1.29 | −1.18 | −1.13 | 1.05 |
| **5-Caf-qui** | 1.27E−08 | 1.89 | −1.17 | 2.06 | −2.21 | 1.09 | 2.41 |
| **4-Caf-qui** | 1.10E−08 | 2.99 | 2.74 | 5.85 | −1.09 | 1.96 | 2.13 |
| **Pro-B1** | 1.71E−09 | 4.43 | −1.08 | 10.13 | −4.79 | 2.28 | 10.94 |
| **Cat** | 2.03E−07 | 2.47 | −1.04 | 4.55 | −2.56 | 1.84 | 4.72 |
| **Epi** | 1.29E−03 | 1.49 | 1.10 | 3.21 | −1.36 | 2.15 | 2.93 |
| **Q-gal** | 7.63E−06 | −1.39 | −4.44 | −2.61 | −3.19 | −1.87 | 1.70 |
| **Q-glu** | 9.43E−07 | −2.04 | −3.80 | −4.60 | −1.87 | −2.26 | −1.21 |
| **K-rut** | 7.12E−06 | 1.07 | −2.66 | −2.45 | −2.86 | −2.63 | 1.09 |

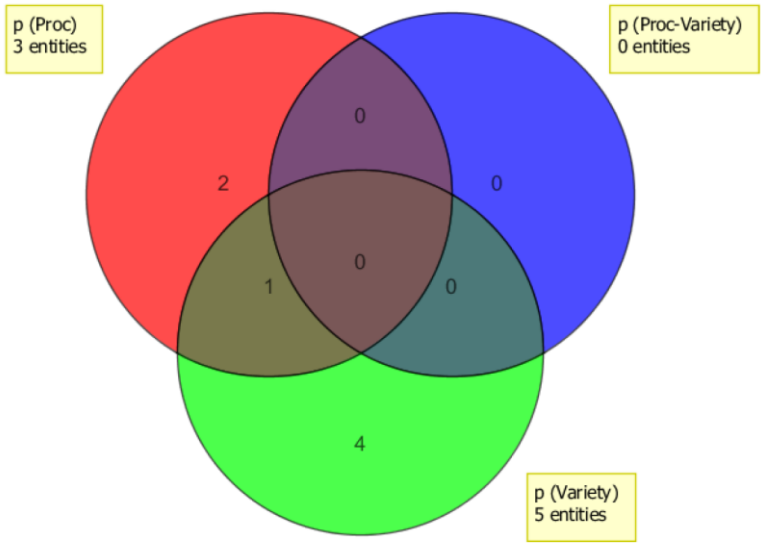
**Pear juices samples**

Oneway Anova p-value cut-off:.0.05

| Compound | p | FC ([Alej] vs [Blanq]) | FC ([Alej] vs [Conf]) | FC ([Blanq] vs [Conf]) |
|---|---|---|---|---|
| **SUCR** | 1.68E−10 | −1.83 | −4.44 | −2.43 |
| **aGLUC** | 4.09E−05 | 1.75 | 1.49 | −1.17 |
| **bGLUC** | 4.54E−03 | 1.62 | 1.22 | −1.33 |
| **FRUCT** | 7.30E−03 | −1.24 | 1.10 | 1.37 |
| **ASP** | 4.36E−08 | −3.38 | −1.30 | 2.61 |
| **MA** | 4.33E−04 | −1.55 | −1.07 | 1.44 |
| **QA** | 3.93E−08 | −1.33 | 2.16 | 2.89 |
| **ALA** | 5.18E−06 | −1.67 | 1.55 | 2.58 |
| **Arb** | 3.25E−10 | 2.28 | 1.86 | −1.22 |
| **ProCat-glu** | 1.64E−15 | 2.70 | 5.22 | 1.93 |
| **3-Caf-qui** | 4.02E−13 | 3.01 | 3.81 | 1.26 |
| **Cou-hex** | 6.40E−20 | 3.56 | 11.44 | 3.21 |
| **5-Caf-qui** | 2.88E−04 | 1.39 | 1.44 | 1.03 |
| **4-Caf-qui** | 1.32E−13 | 2.92 | 3.30 | 1.13 |
| **Pro-B2** | 3.21E−10 | 2.44 | 2.52 | 1.03 |
| **Epi** | 8.23E−10 | 2.40 | 2.63 | 1.10 |
| **Q-rut** | 3.35E−10 | 1.22 | 9.08 | 7.46 |
| **Q-gal** | 9.36E−11 | −1.97 | 1.39 | 2.74 |
| **Q-glu** | 1.12E−07 | −1.76 | −1.00 | 1.75 |
| **Iso-rob** | 4.26E−12 | 5.24 | 3.23 | −1.62 |
| **Iso-rut** | 4.66E−11 | 6.33 | 1.60 | −3.96 |
| **Iso-gal** | 7.60E−15 | 5.81 | 1.52 | −3.83 |
| **Iso-glu** | 3.14E−13 | 3.73 | −1.27 | −4.75 |

**Venn Diagram Report**

Experiment : NMR-Peach
Active entity list : All Entities



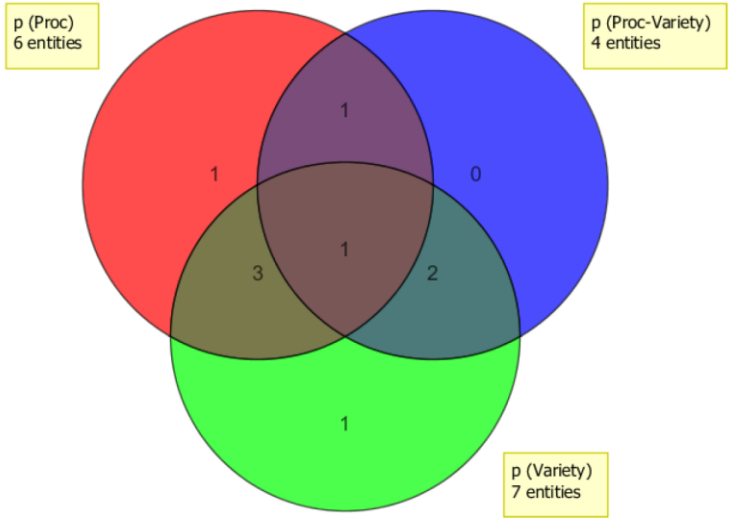

Description
VennDiagram for sets:
p (Proc)
p (Proc-Variety)
p (Variety)

Venn Colors

| |
|---|
| p (Proc) |
| p (Proc-Variety) |
| p (Variety) |

**Venn Diagram Report**

Experiment : Poly-Peach
Active entity list : Oneway ANOVA p cut-off = 0.05




Description
VennDiagram for sets:
p (Proc)
p (Proc-Variety)
p (Variety)

Venn Colors

| |
|---|
| p (Proc) |
| p (Proc-Variety) |
| p (Variety) |