# Figure S2. Supervised O2PLS-DA of NMR and HPLC-DAD data matrices for apples and pears


a) Apples, NMR dataset, O2PLS-DA score plots, 5+3 model
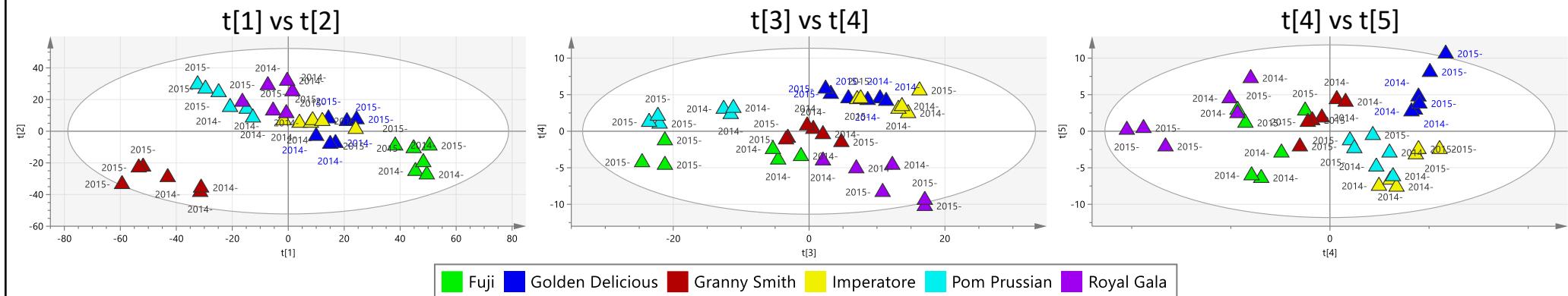
b) Apples, NMR dataset, O2PLS-DA loading plots, 5+3 model
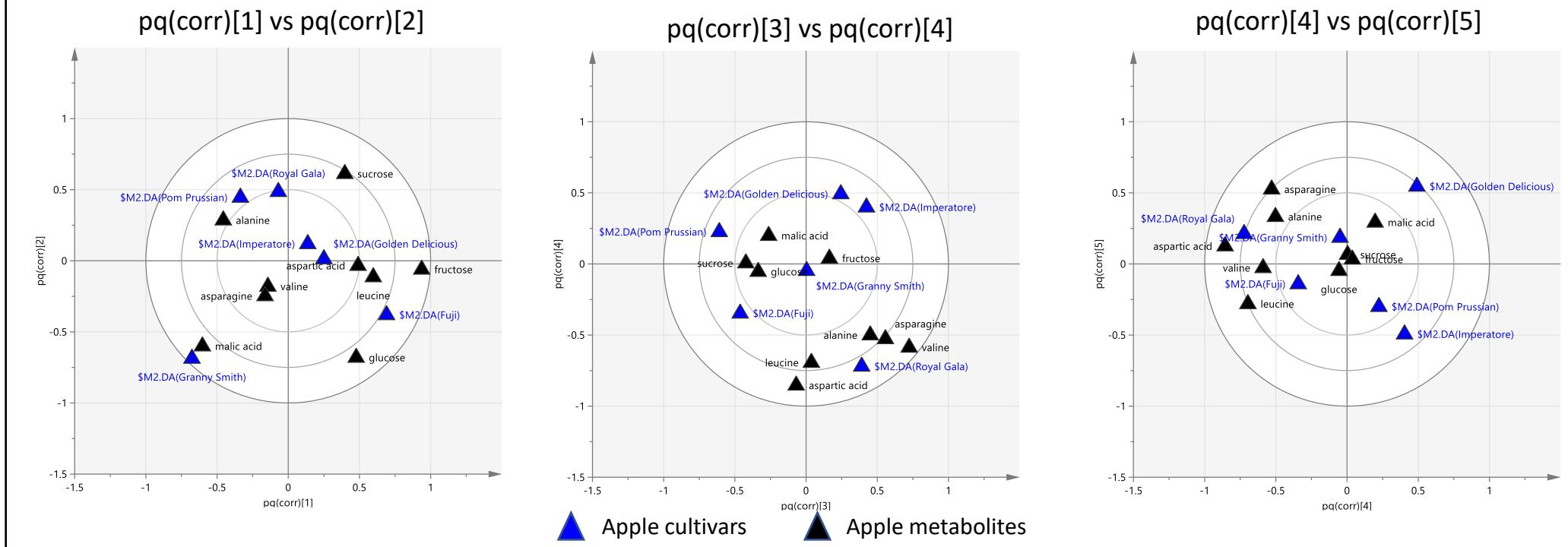
c) Apples, HPLC-DAD dataset, O2PLS-DA score plots, 5+2 model

t[1] vs t[2]

t[3] vs t[4]

t[4] vs t[5]

Legend: Fuji | Golden Delicious | Granny Smith | Imperatore | Pom Prussian | Royal Gala
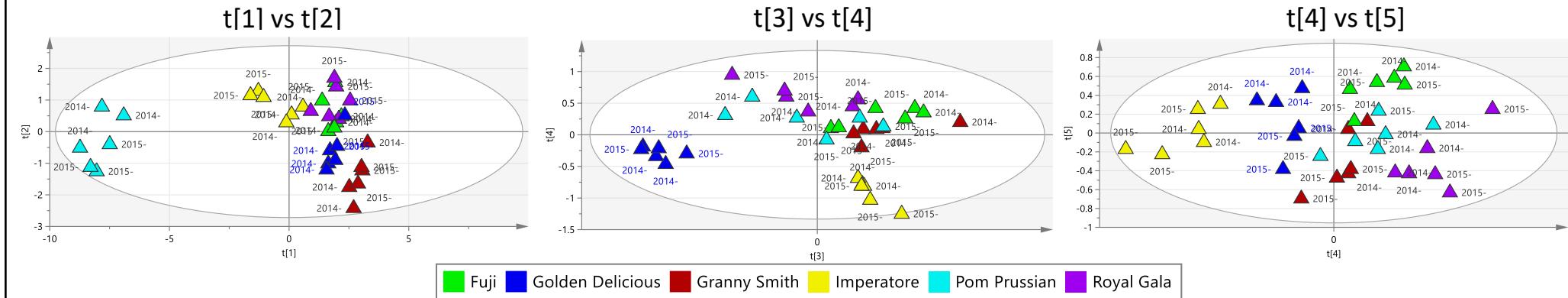
d) Apples, HPLC-DAD dataset, O2PLS-DA loading plots, 5+2 model

pq(corr)[1] vs pq(corr)[2]

pq(corr)[3] vs pq(corr)[4]

pq(corr)[4] vs pq(corr)[5]

Apple cultivars   Apple metabolites
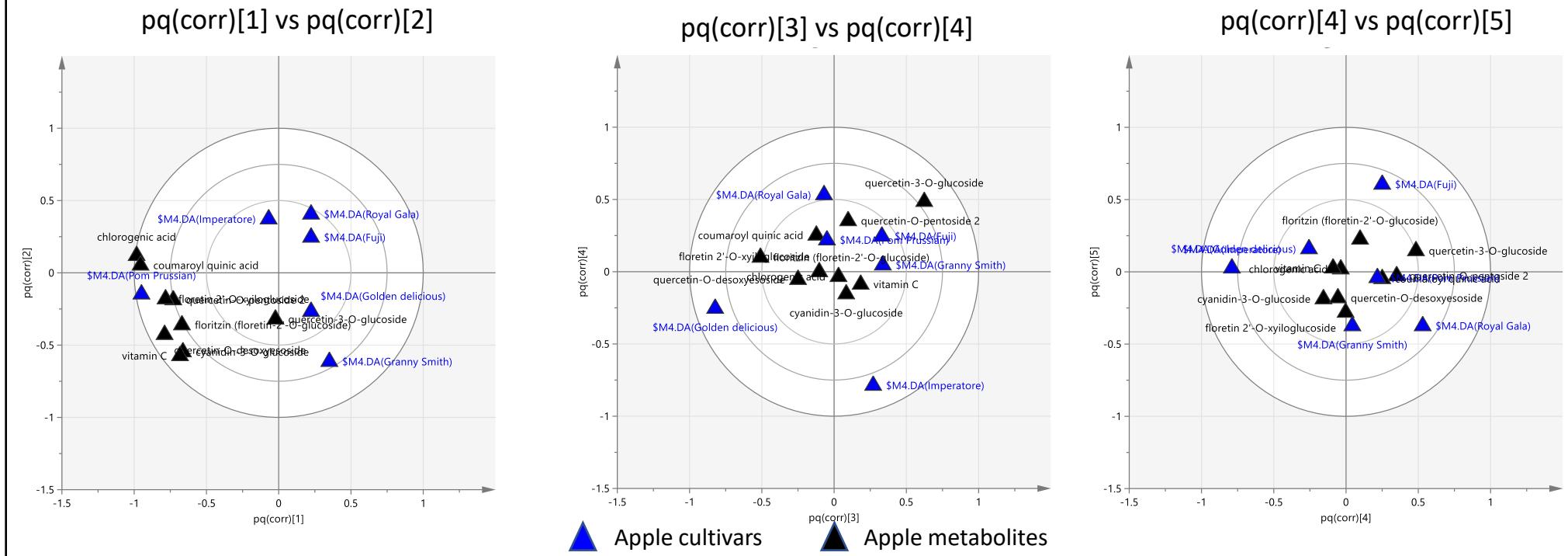
e) Pears, NMR dataset, O2PLS-DA score plot, 5+3 model

t[1] vs t[2]

t[1] vs t[3]

Abate   Conference   Decana   Kaiser   Williams
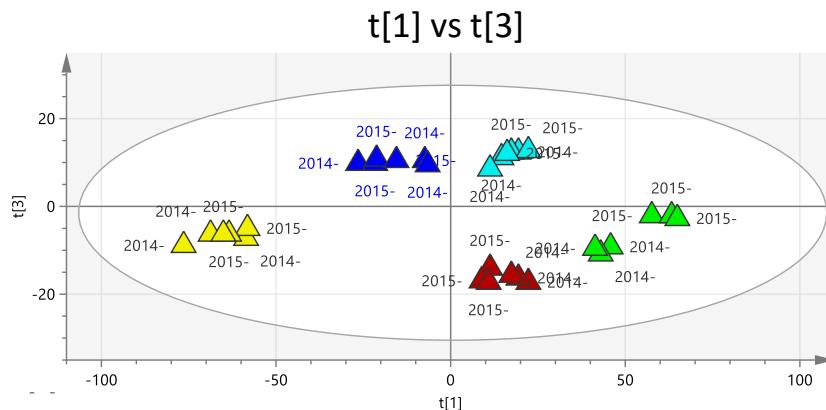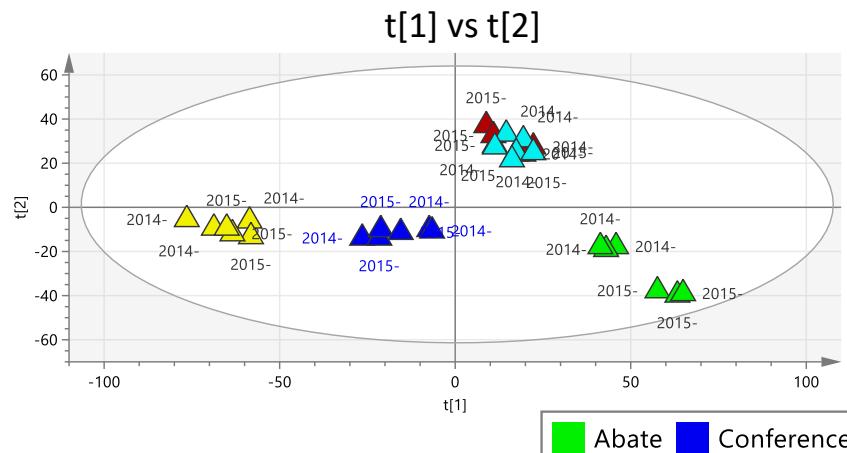
f) Pears, NMR dataset, O2PLS-DA loading plot, 5+3 model

pq(corr)[1] vs pq(corr)[2]

pq(corr)[1] vs pq(corr)[3]

Pear cultivars   Pear metabolites
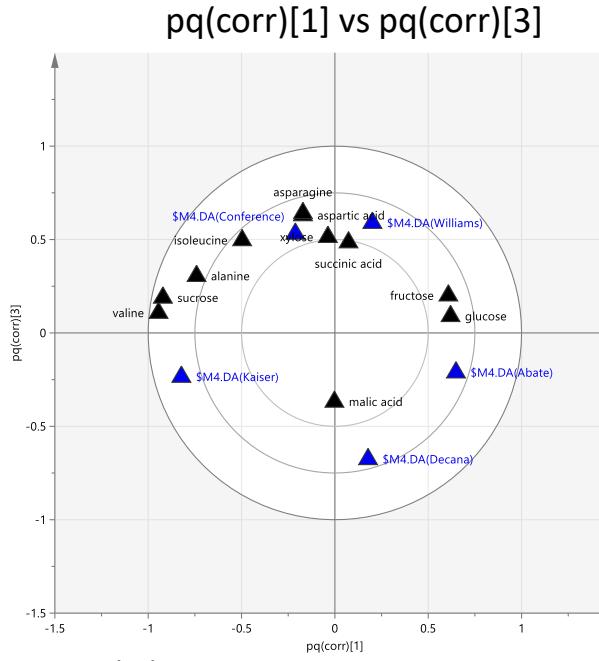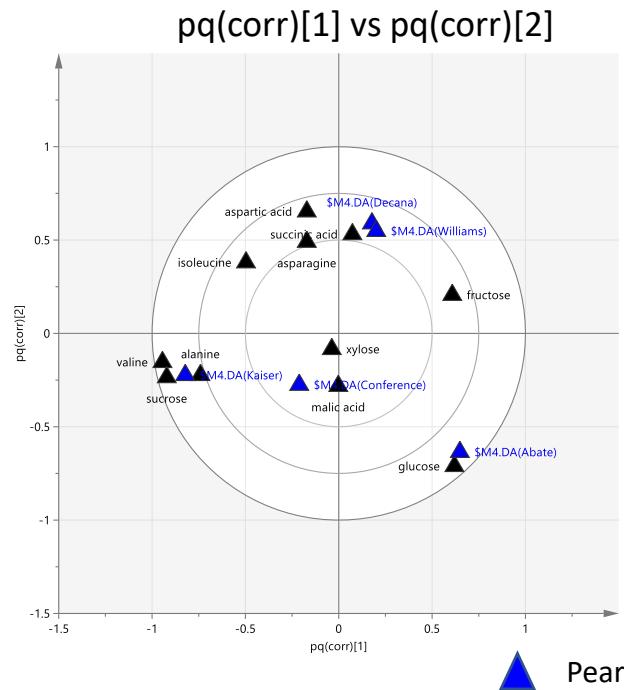
g) Pears, HPLC-DAD dataset, O2PLS-DA score plot, 5+2 model

t[1] vs t[2]

t[3] vs t[4]

| Abate | Conference | Decana | Kaiser | Williams |
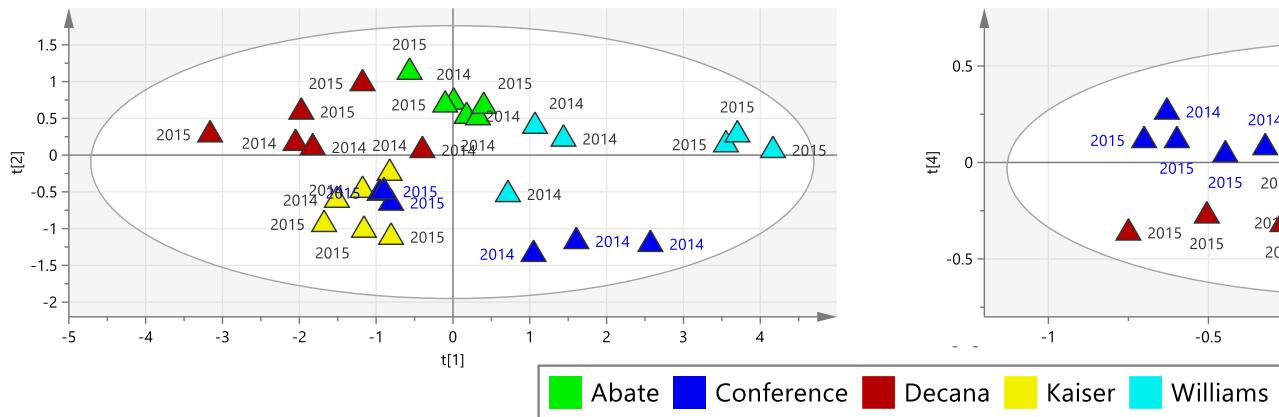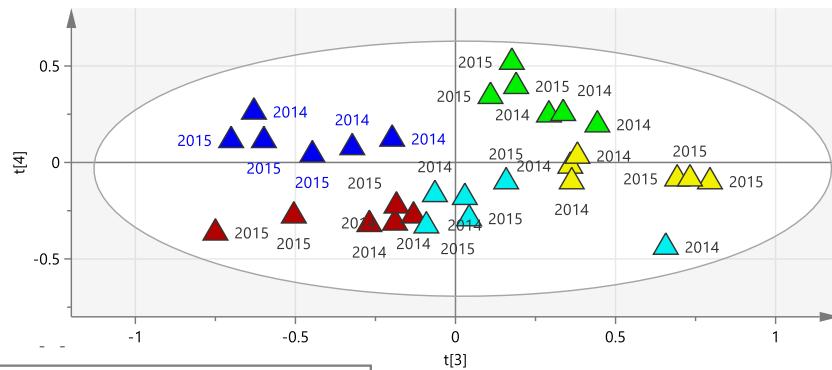
h) Pears, HPLC-DAD dataset, O2PLS-DA loading plot, 5+2 model

pq(corr)[1] vs pq(corr)[2]

pq(corr)[3] vs pq(corr)[4]

Pear cultivars   Pear metabolites
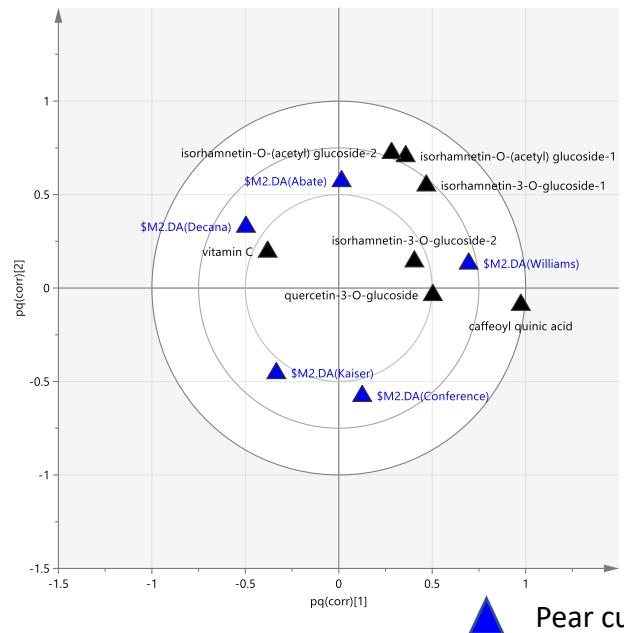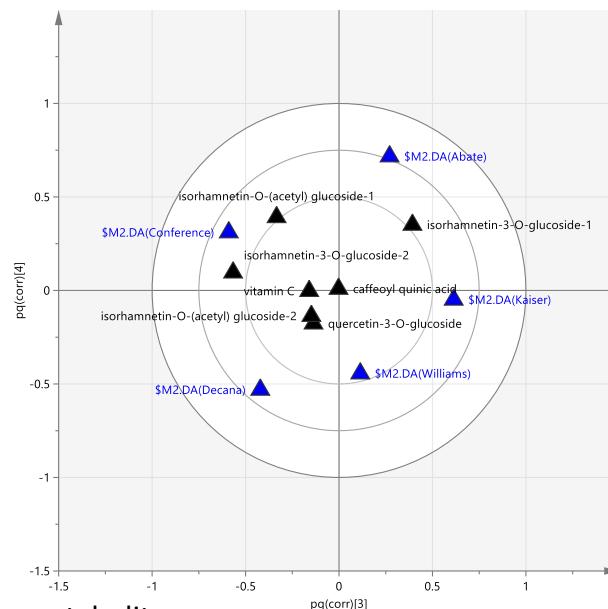
i) Pears, HPLC-DAD and NMR datasets, O2PLS-DA score plot, 1+1model
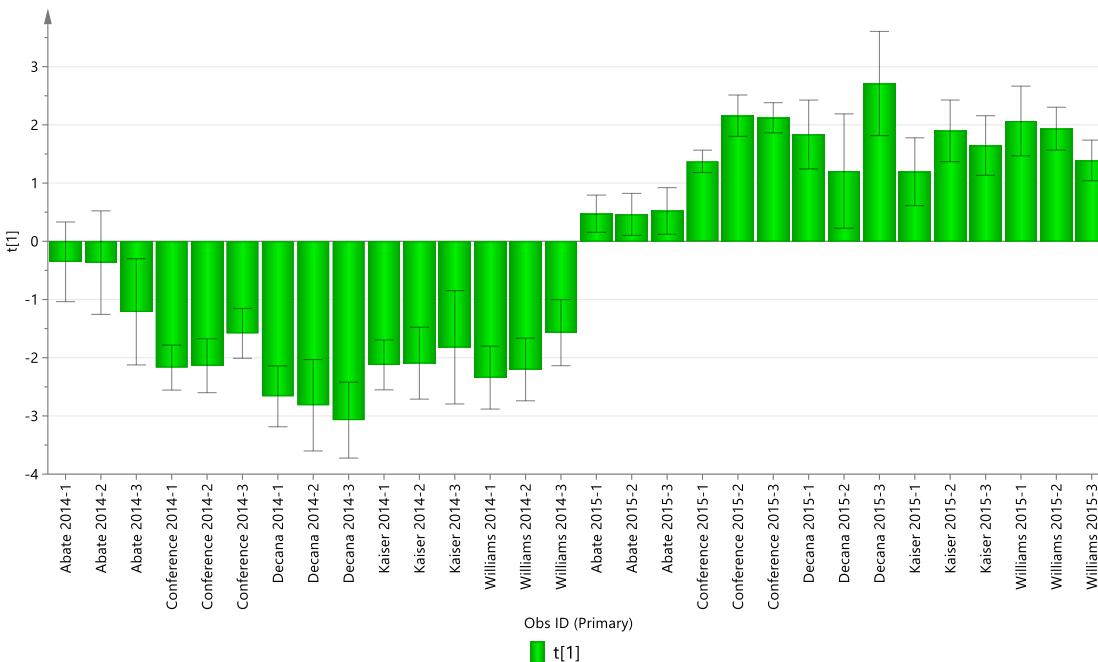
j) Pears, HPLC-DAD and NMR datasets, O2PLS-DA loading plot, 1+1model