Additional file 4: Metabolite eigenvalues for principal component analysis (PCA). The metabolites appear below are the seven metabolites with the highest eigenvalues for components one and two, in each of the PCAs performed for GC-MS and UPLC-QTOF-MS/MS data sets, for both fruit pulp and seed tissues. The values in parentheses represent the *m/z* for each metabolite. MP = main product, BP = by product

PCA of GC-MS data set obtained from fruit pulp tissues			
Metabolite	**Component 1**	**Metabolite**	**Component 2**
Glucose MP	3.665	***myo*-Inositol**	4.918
Fructose MP	3.200	**Glucose MP**	2.403
***myo*-Inositol**	3.162	**Fructose MP**	1.156
Fructose BP	2.141	**Fructose BP**	1.043
Glucose BP	0.874	**Citrate**	0.968
Citrate	0.168	**Glucose BP**	0.822
Proline	0.027	**Malate**	0.081
PCA of GC-MS data set obtained from seed tissues			
Metabolite	**Component 1**	**Metabolite**	**Component 2**
***myo*-Inositol**	5.406	**Sucrose**	4.831
Sucrose	1.862	**Raffinose**	2.218
Glucose MP	1.271	***myo*-Inositol**	1.743
Fructose MP	1.211	**Glucose MP**	1.447
Fructose BP	0.869	**Citrate**	0.801
Raffinose	0.182	**Fructose MP**	0.185
Citrate	0.181	**Pyroglutamate**	0.126
PCA of UPLC-QTOF-MS/MS data set obtained from fruit pulp tissues			
Metabolite	**Component 1**	**Metabolite**	**Component 2**
NA (160.0756)	2.379	**NA (188.0665)**	2.329
Hylocerenin (695.1955)	1.604	**Hylocerenin (695.1955)**	1.540
NA (151.0348)	1.132	**NA (160.0756)**	1.058
Phylocactin (637.1495)	0.645	**NA (151.0348)**	0.810
NA (188.0665)	0.396	**Phylocactin (637.1495)**	0.688
NA (127.0351)	0.353	**NA (127.0351)**	0.405
NA (551.1488)	0.322	**NA (551.1488)**	0.403
PCA of UPLC-QTOF-MS/MS data set obtained from seed tissues			
Metabolite	**Component 1**	**Metabolite**	**Component 2**
NA (188.0699)	3.354	**NA (285.0811)**	3.282
NA (285.0811)	1.982	**NA (188.0699)**	1.798
NA (160.0657)	1.788	**NA (329.9262)**	1.022
NA (149.0581)	0.614	**NA (149.0581)**	0.823
NA (493.2780)	0.587	**NA (147.0416)**	0.771
NA (147.0416)	0.539	**NA (160.0657)**	0.448
NA (365.1045)	0.530	**NA (151.0308)**	0.388