Supplementary Table 1: This table reports the two MRM methods, here expressed as method 1 for the negative MRM and method 2 for the positive MRM exploited for TVE quantitative analysis. For each metabolite the following parameters are reported: Declustering Potential (DP), Entrance Potential (EP), Collision Energy (CE), and Collision Cell Exit Potential (CXP).

MRM methods exploited for TVE quantitative analysis							
Compound	**Method**	**Q1 (m/z)**	**Q3 (m/z)**	**DP (V)**	**EP (V)**	**CE (V)**	**CXP (V)**
Allantoin_1	1	157.00	114.00	-25	-14	-10	-13
Allantoin_2	1	157.00	140.00	-25	-14	-10	-13
S-cis-abscissic acid_1	1	263.00	153.00	-20	-10	-10	-13
S-cis-abscissic acid_2	1	263.00	219.00	-20	-10	-10	-13
Ferulic acid D-glucoside_1	1	355.00	193.00	-55	-6	-19	-44
Ferulic acid D-glucoside_2	1	355.00	175.00	-55	-6	-19	-44
Jasmonic acid_1	1	209.00	59.00	-60	-7	-20	-12
Jasmonic acid_2	1	209.00	109.00	-60	-7	-20	-12
Jasmonic acid_3	1	209.00	165.00	-60	-7	-20	-12
Luteolin_1	1	285.00	133.00	-25	-10	-37	-13
Luteolin_2	1	285.00	151.00	-25	-10	-37	-13

3-(4-hydroxy-3-methoxyphenil) propionic acid	1	195.00	135.90	-100	-11	-22	-7
2,6-dimethoxy-benzoquinone imine derivative_1	2	282.00	223.00	30	10	30	12
2,6-dimethoxy-benzoquinone imine derivative_2	2	282.00	195	30	10	30	12
2,6-dimethoxy-benzoquinone imine derivative_3	2	282.00	100	30	10	30	12
2-methoxy-benzoquinone imine derivative_1	2	183.12	183.12	30	10	30	12
2-methoxy-benzoquinone imine derivative_2	2	183.12	307.24	30	10	30	12
2-methoxy-benzoquinone imine derivative_3	2	183.12	293.24	30	10	30	12

Supplementary Table 2: The correlation values of the calibration curves, obtained from the quantification of the best transition for each molecule, are here reported to infer the MRM methods linearity.

Linearity of the quantified metabolites			
Compound	**Q1 (m/z)**	**Q3 (m/z)**	**Linearity (R^2)**
Allantoin	157.00	114.00	0.9844
S-cis-abscissic acid	263.00	153.00	0.9792
Ferulic acid D-glucoside	355.00	193.00	0.9901
Jasmonic acid	209.00	59.00	0.9956
Luteolin	285.00	133.00	0.9911
3-(4-hydroxy-3-methoxyphenil) propionic acid	195.00	135.90	0.9961
2,6-dimethoxy-benzoquinone imine derivative	282.00	223.00	0.9977
2-methoxy-benzoquinone imine derivative	183.12	183.12	0.9433