

Table S1. Optimized MRM transitions for MS/MS detection on Xevo TQ-XS Mass spectrometric system with argon collision gas.

Analyte and transition order	Q1 m/z	Q3 m/z	cone voltage (V)	Collision Energy (eV)	RT (mins)	polarity	Used for quantitation
Absciscic Acid 1	263.1	153.0	20	10	7.13	US neg	YES
Absciscic Acid 2	263.1	204.0	20	20	7.13	US neg	
Absciscic Acid 3	263.1	201.1	20	18	7.13	US neg	
Absciscic Acid 4	263.1	219.1	20	12	7.13	US neg	
[² H ₆] Absciscic Acid	269.1	159.0	20	10	7.10	US neg	YES
Dihydrophaseic Acid 1	281.1	237.2	25	12	3.49	US neg	YES
Dihydrophaseic Acid 2	281.1	171.1	25	18	3.49	US neg	
Dihydrophaseic Acid 3	281.1	123.1	25	18	3.49	US neg	
Indole-3-acetic acid 1	176.1	130.1	25	14	5.97	US pos	YES
Indole-3-acetic acid 2	176.1	103.1	25	34	5.97	US pos	
Indole-3-acetic acid 3	176.1	77.1	25	50	5.97	US pos	
Phaseic Acid 1	279.1	139.0	25	12	5.13	US neg	YES
Phaseic Acid 2	279.1	205.2	25	14	5.13	US neg	
Phaseic Acid 3	279.1	168.2	25	14	5.13	US neg	
p-Hydroxybenzoic Acid 1	137.0	93.0	20	12	2.83	US neg	YES
p-Hydroxybenzoic Acid 2	137.0	64.9	20	24	2.83	US neg	
Salicylic Acid 1	137.0	93.0	20	12	5.82	US neg	YES
Salicylic Acid 2	137.0	64.9	20	24	5.82	US neg	