

## Supporting Information

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# Phenolic Compounds of *Pinus brutia* Ten.: Chemical Investigation and Quantitative Analysis Using an Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry with Electrospray Ionization Source

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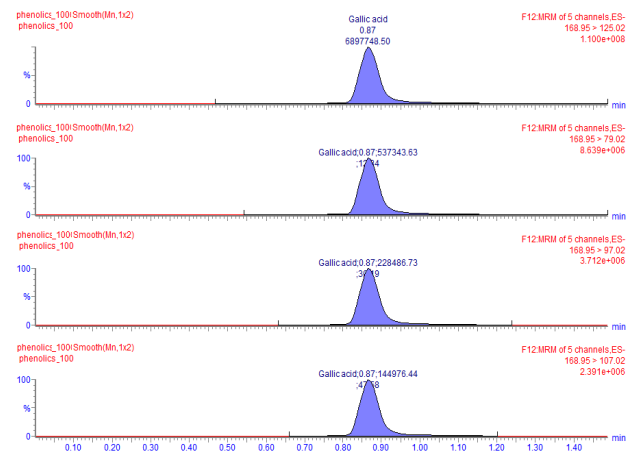
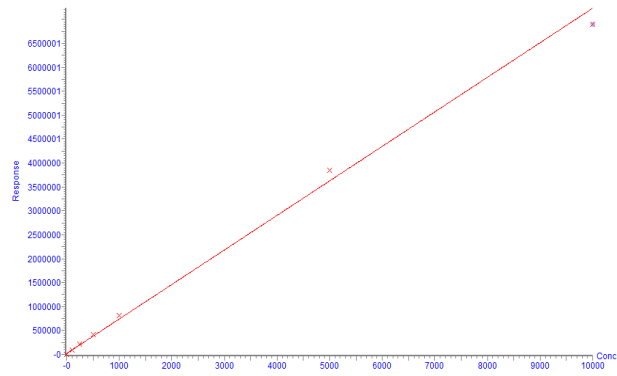
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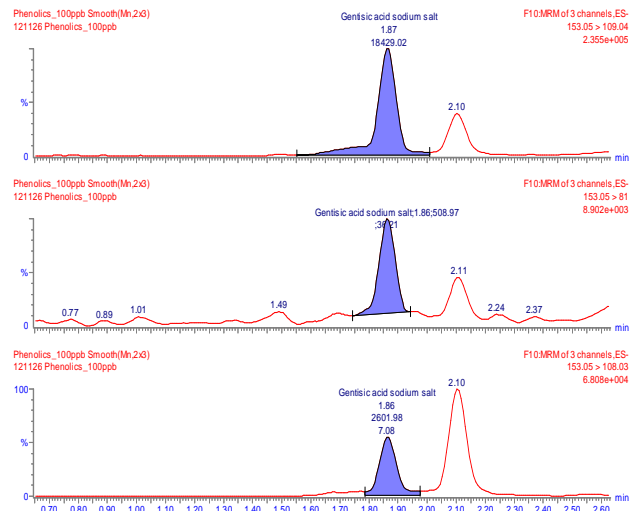
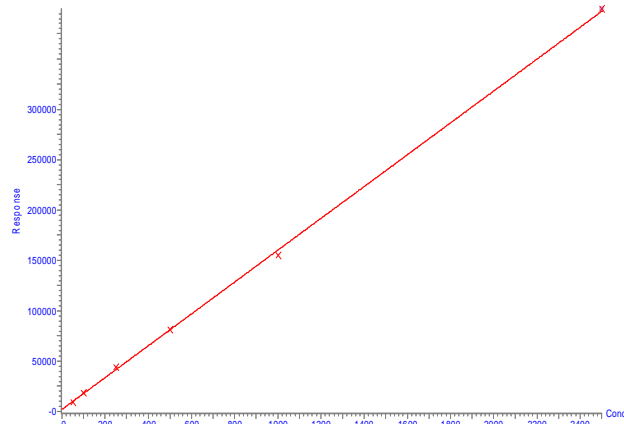
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Compound name: Gallic acid  
 Correlation coefficient:  $r = 0.997972$ ,  $r^2 = 0.995948$   
 Calibration curve:  $721.654 \cdot x + 19597$   
 Response type: External Std. Area  
 Curve type: Linear, Origin, Exclude, Weighting: 1/x, Axis trans: None



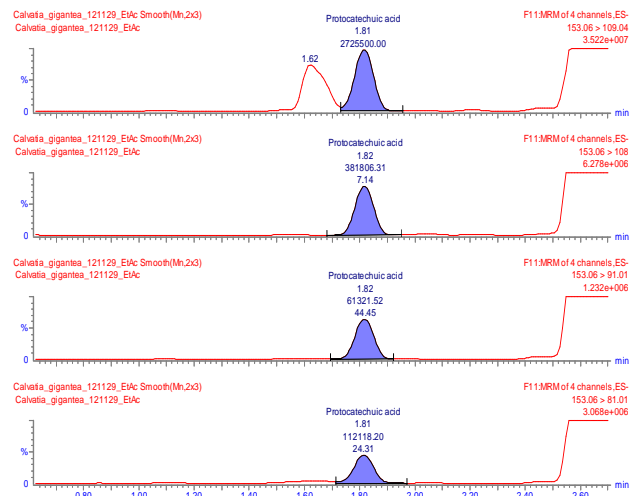
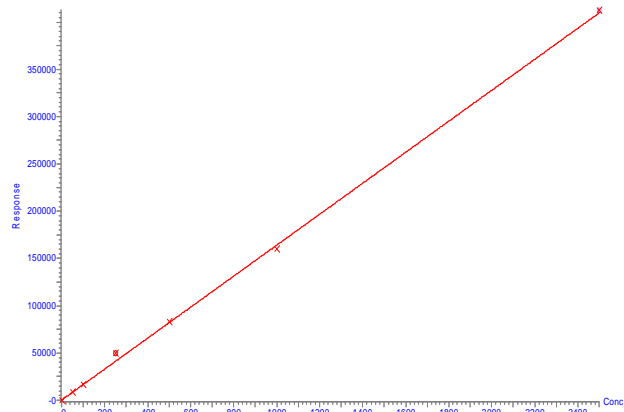
### S1: Calibration Curve and UPLC-MS/MS Chromatogram of Gallic acid

Compound name: Gentisic acid sodium salt  
 Correlation coefficient:  $r = 0.998669$ ,  $r^2 = 0.998339$   
 Calibration curve:  $158.025 \cdot x + 2143.53$   
 Response type: External Std. Area  
 Curve type: Linear, Origin, Exclude, Weighting: 1/x, Axis trans: None



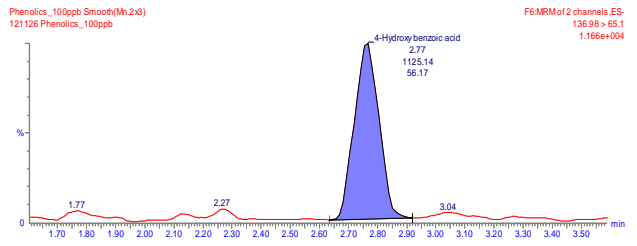
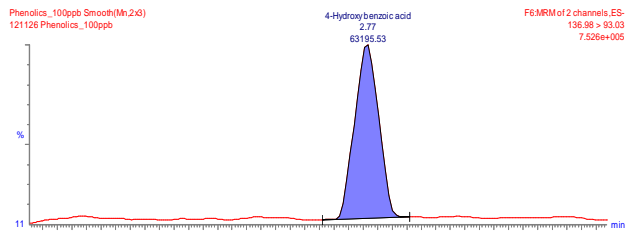
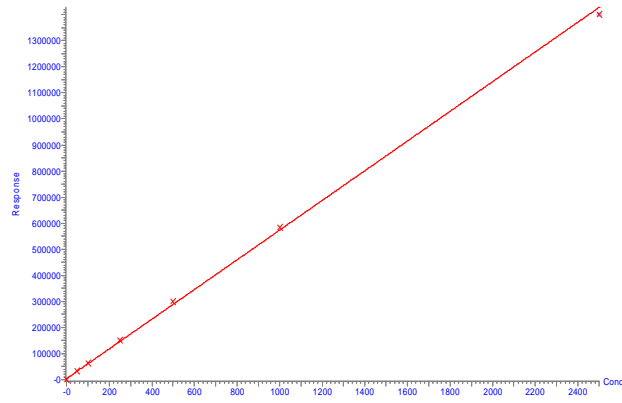
### S2: Calibration Curve and UPLC-MS/MS Chromatogram of Gentisic acid

Compound name: Protocatechuic acid  
 Correlation coefficient:  $r = 0.998858$ ,  $r^2 = 0.999716$   
 Calibration curve:  $163.811 \cdot x + 269.959$   
 Response type: External Std. Area  
 Curve type: Linear, Origin, Exclude, Weighting: 1/x, Axis trans: None



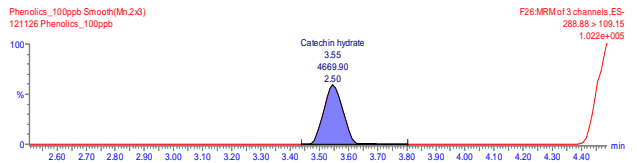
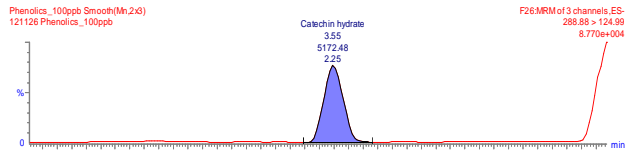
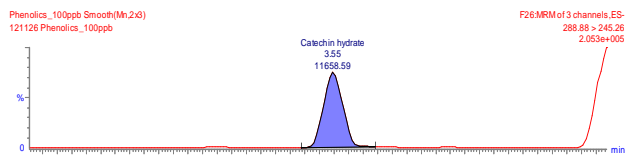
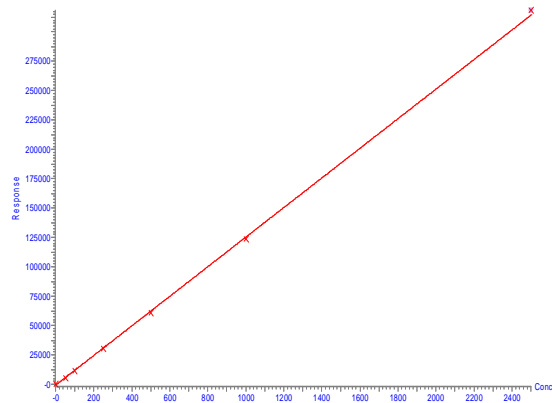
### S3: Calibration Curve and UPLC-MS/MS Chromatogram of Protocatechuic acid

Compound name: 4-Hydroxybenzoic acid  
 Correlation coefficient:  $r = 0.999593$ ,  $r^2 = 0.999187$   
 Calibration curve:  $569.645 \cdot x + 3815.13$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



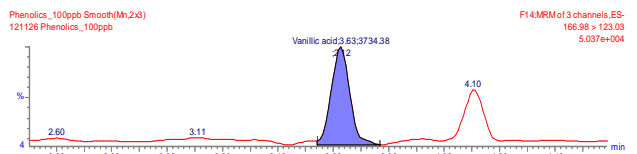
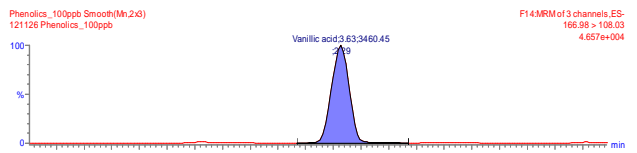
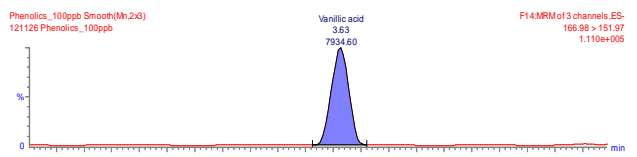
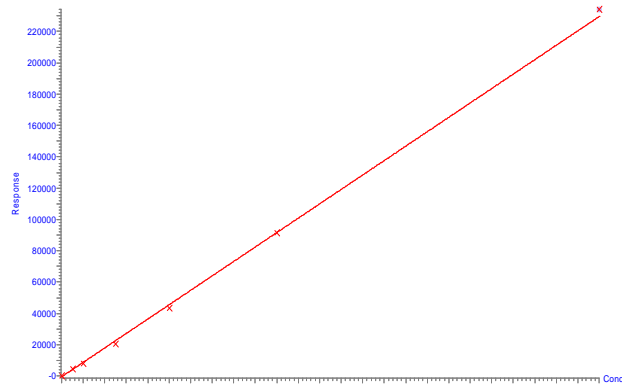
**S4: Calibration Curve and UPLC-MS/MS Chromatogram of 4-hydroxy benzoic acid**

Compound name: Catechin hydrate  
 Correlation coefficient:  $r = 0.999745$ ,  $r^2 = 0.999489$   
 Calibration curve:  $126.014 \cdot x + 483.675$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



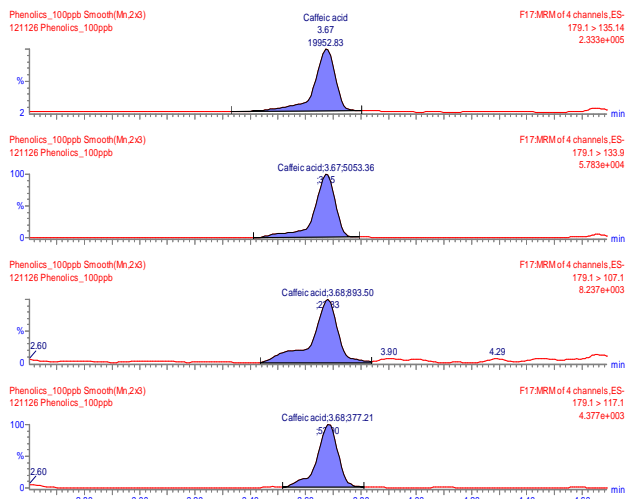
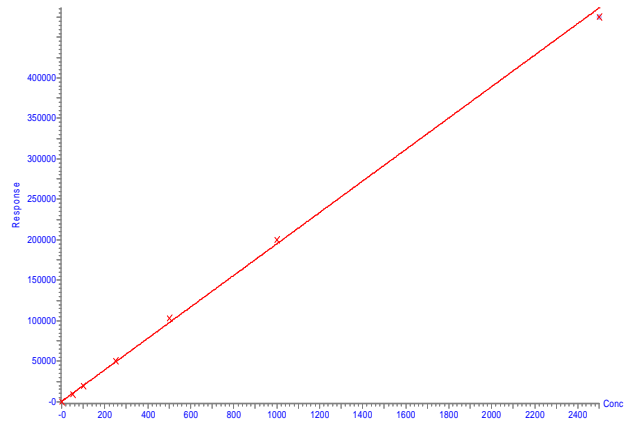
**S5: Calibration Curve and UPLC-MS/MS Chromatogram of Catechin hydrate**

Compound name: Vanillic acid  
 Correlation coefficient:  $r = 0.999226$ ,  $r^2 = 0.998452$   
 Calibration curve:  $92.3129 \cdot x + 393.299$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



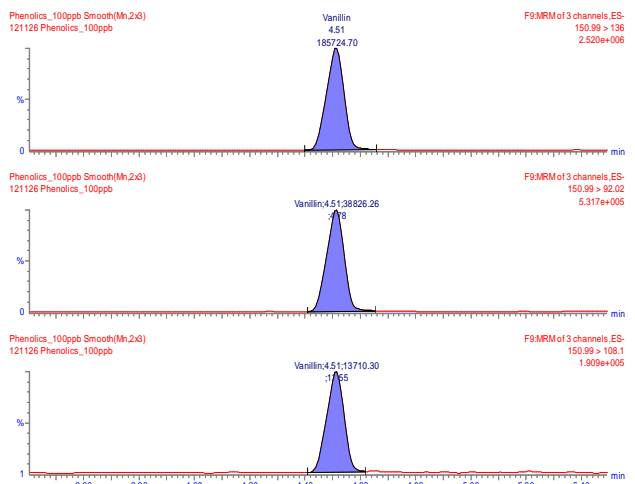
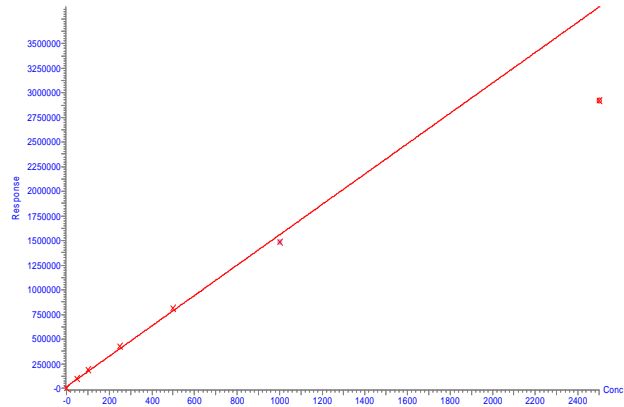
**S6: Calibration Curve and UPLC-MS/MS Chromatogram of Vanillic acid**

Compound name: Caffeic acid  
 Correlation coefficient:  $r = 0.999451$ ,  $r^2 = 0.998902$   
 Calibration curve:  $194.377 \cdot x + 585.655$   
 Response type: External Std. Area  
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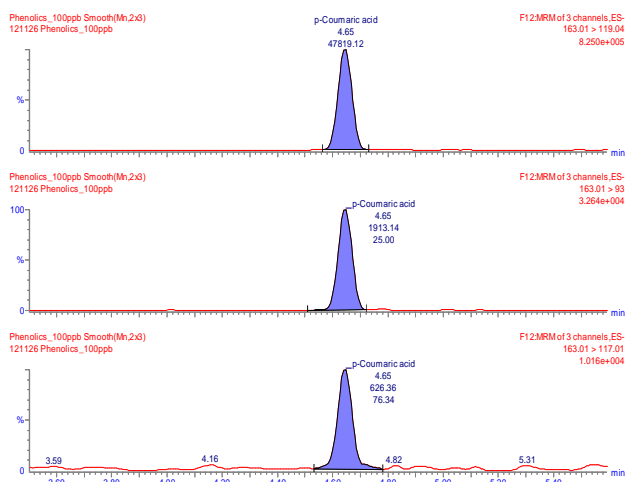
**S7: Calibration Curve and UPLC-MS/MS Chromatogram of Caffeic acid**

Compound name: Vanillin  
 Correlation coefficient:  $r = 0.997494$ ,  $r^2 = 0.994994$   
 Calibration curve:  $1542.35 \cdot x + 16268.9$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



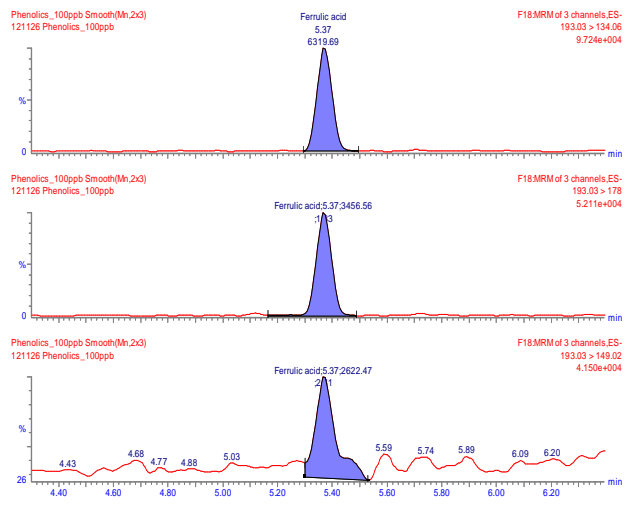
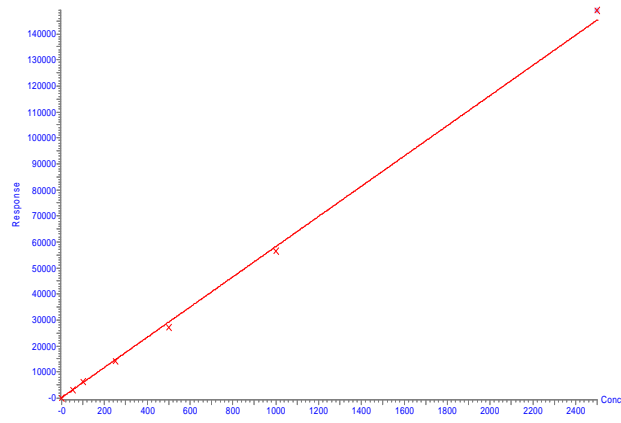
**S8: Calibration Curve and UPLC-MS/MS Chromatogram of Vanillin**

Compound name: p-Coumaric acid  
 Correlation coefficient:  $r = 0.999447$ ,  $r^2 = 0.998894$   
 Calibration curve:  $499.659 \cdot x + 1449.58$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



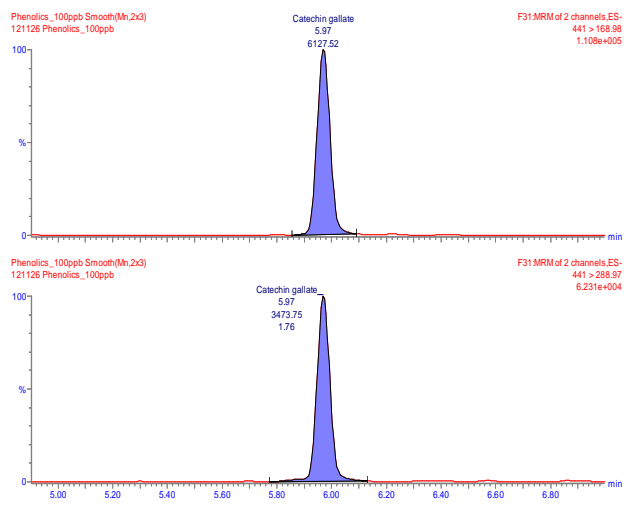
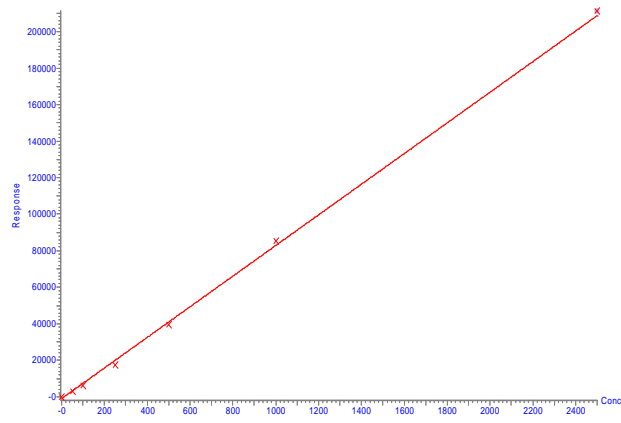
**S9: Calibration Curve and UPLC-MS/MS Chromatogram of p-Coumaric acid**

Compound name: Ferulic acid  
 Correlation coefficient:  $r = 0.999204$ ,  $r^2 = 0.998408$   
 Calibration curve:  $58.0716 \cdot x + 168.08$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



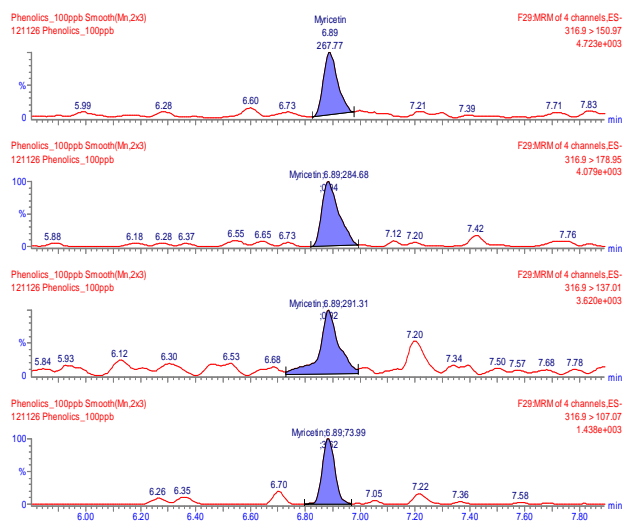
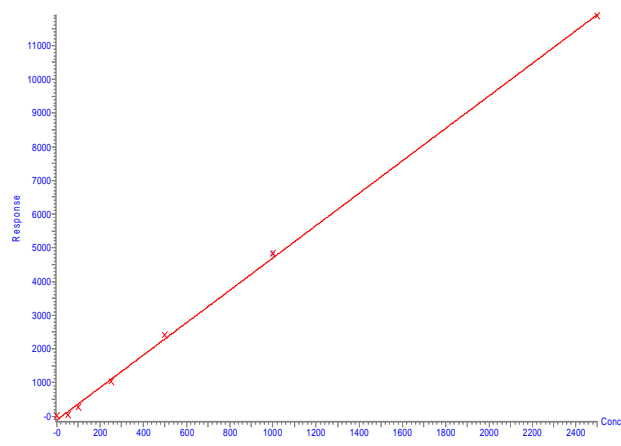
### S10: Calibration Curve and UPLC-MS/MS Chromatogram of Ferulic acid

Compound name: Catechin gallate  
 Correlation coefficient:  $r = 0.998647$ ,  $r^2 = 0.997295$   
 Calibration curve:  $93.858 \cdot x + 998.732$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



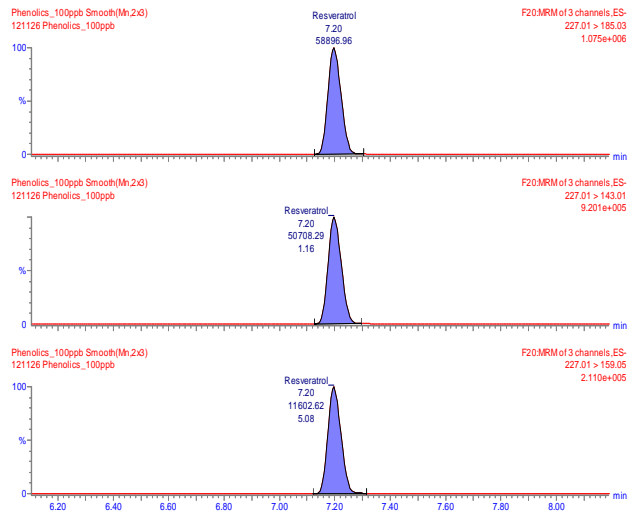
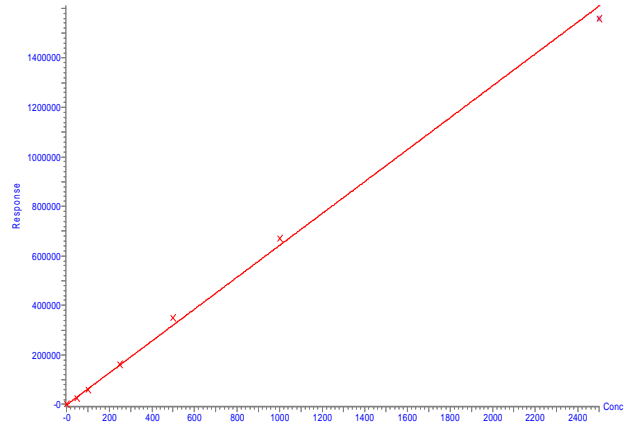
### S11: Calibration Curve and UPLC-MS/MS Chromatogram of Catechin gallate

Compound name: Myricetin  
 Correlation coefficient:  $r = 0.996763$ ,  $r^2 = 0.993537$   
 Calibration curve:  $4.81109 \cdot x + 114.559$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



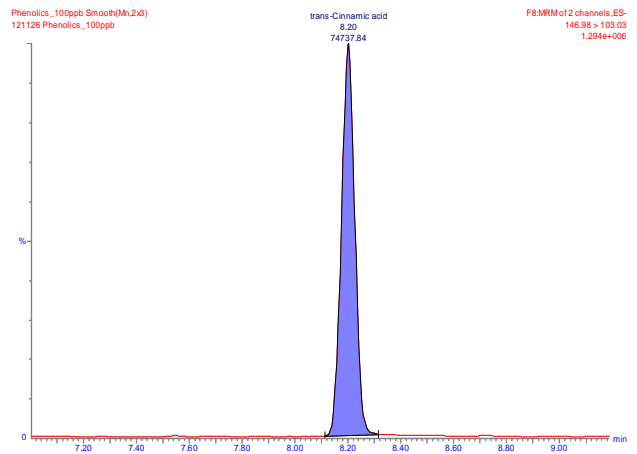
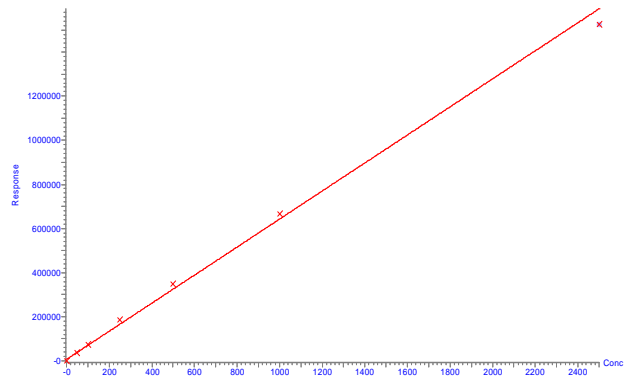
### S12: Calibration Curve and UPLC-MS/MS Chromatogram of Myricetin

Compound name: Resveratrol  
 Correlation coefficient:  $r = 0.998737$ ,  $r^2 = 0.997475$   
 Calibration curve:  $644.743 \cdot x + -1890.26$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



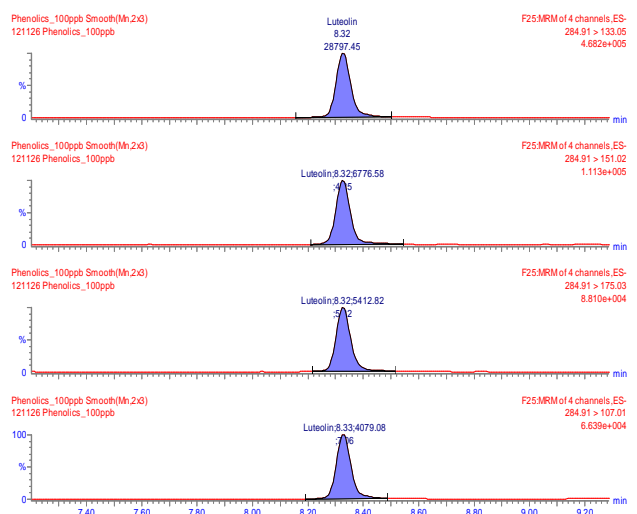
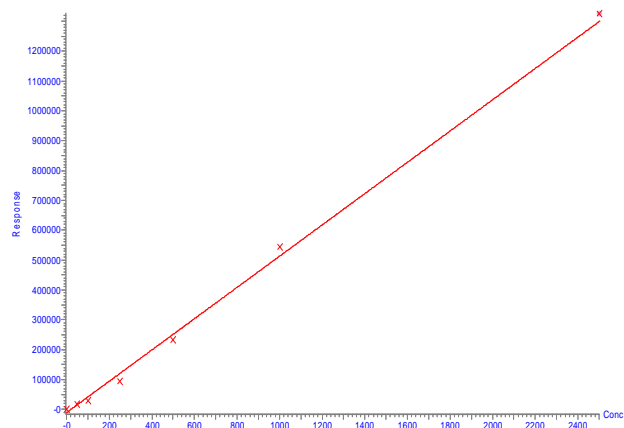
**S13: Calibration Curve and UPLC-MS/MS Chromatogram of Resveratrol**

Compound name: *trans*-Cinnamic acid  
 Correlation coefficient:  $r = 0.997789$ ,  $r^2 = 0.995543$   
 Calibration curve:  $635.856 \cdot x + 7144.66$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



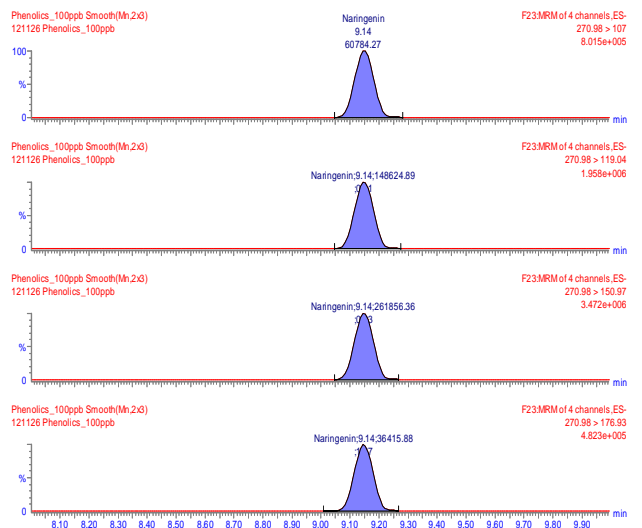
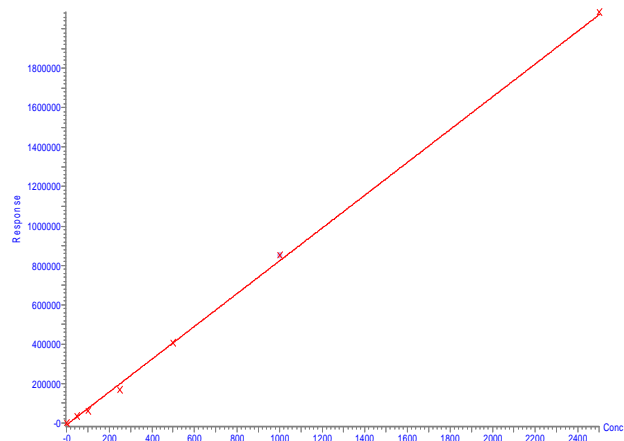
**S14: Calibration Curve and UPLC-MS/MS Chromatogram of *trans*-Cinnamic acid**

Compound name: Luteolin  
 Correlation coefficient:  $r = 0.995902$ ,  $r^2 = 0.991821$   
 Calibration curve:  $523.933 \cdot x + -10639.1$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



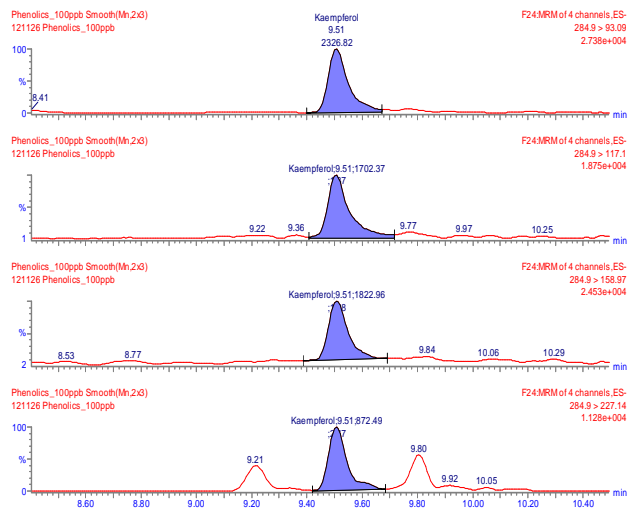
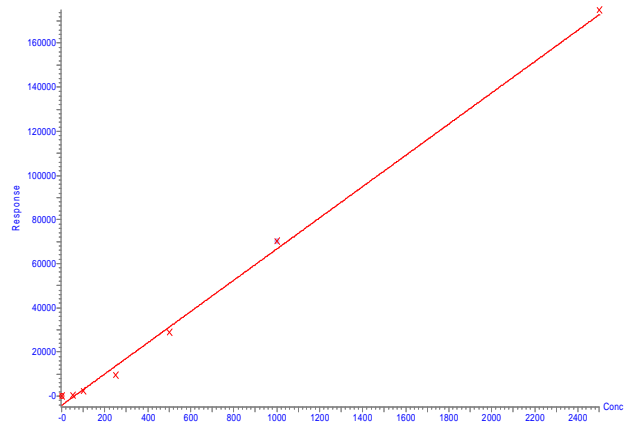
**S15: Calibration Curve and UPLC-MS/MS Chromatogram of Luteolin**

Compound name: Naringenin  
 Correlation coefficient:  $r = 0.998526$ ,  $r^2 = 0.997055$   
 Calibration curve:  $832.386 \cdot x + 9156.81$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



**S16: Calibration Curve and UPLC-MS/MS Chromatogram of Naringenin**

Compound name: Kaempferol  
 Correlation coefficient:  $r = 0.996520$ ,  $r^2 = 0.993051$   
 Calibration curve:  $70.8133 \cdot x + 4171.65$   
 Response type: External Std. Area  
 Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



**S17: Calibration Curve and UPLC-MS/MS Chromatogram of Kaempferol**



### S18. Analytical Parameters of the Method

Compound	LOD (mg 100 mL <sup>-1</sup> )	LOQ (mg 100 mL <sup>-1</sup> )	CV% <sup>a</sup>	CV% <sup>b</sup>	Recovery (%) <sup>b</sup>	Stability CV% <sup>c</sup>	Accuracy (%) <sup>d</sup>	Calibration equations	r <sup>2</sup>
4-hydroxy benzoic acid	0.009	0.015	0.003	0.036	85.7-99.6	0.95	95.1-97.6	y=518.823x+12509.1	0.998011
<i>trans</i> -Cinnamic acid	0.003	0.005	0.001	0.011	94.4-98.0	0.43	97.7-100.5	y=697.454x+265.934	0.996617
Resveratrol	0.006	0.010	0.002	0.044	85.5-108.7	1.55	97.1-99.8	y=575.926x+3765.28	0.994946
Catechin gallate	0.018	0.030	0.006	0.096	96.1-100.0	1.04	85.4-98.7	y=115.859x-4152.47	0.993454
Homogentisic acid	0.015	0.025	0.005	0.075	90.2-93.7	1.29	95.1-98.8	y=4.05441x-3.93614	0.995159
Gentisic acid	0.036	0.060	0.012	0.144	98.9-99.9	1.18	98.2-99.9	y=112.964x+4366.91	0.994179
Vanillin	0.021	0.035	0.007	0.091	91.3-94.9	1.17	97.1-99.2	y=1209.68x+17245.9	0.998989
Vanillic acid	0.012	0.020	0.004	0.048	97.9-99.9	1.01	89.6-95.9	y=137.65x+3637.2	0.991877
Catechin hydrate	0.054	0.090	0.018	0.198	98.3-101.7	0.72	97.6-101.5	y=87.4061x+73404.39	0.994509
Chlorogenic acid	0.042	0.070	0.014	0.168	91.5-93.4	1.18	99.1-100.8	y=824.963x+4666.09	0.996764
<i>p</i> -Coumaric acid	0.033	0.055	0.011	0.132	88.0-100.1	0.86	99.1-100.6	y=580.683x-7946.1	0.996035
Ferulic acid	0.030	0.050	0.010	0.150	87.4-96.8	0.65	94.1-99.9	y=86.9682x-3700.24	0.992075
Hesperetin	0.039	0.065	0.013	0.156	90.0-94.1	1.08	96.1-99.9	y=1589.82x-5719.26	0.999487
Chrysin	0.051	0.085	0.017	0.204	98.7-100.5	0.79	95.2-100.6	y=575.5x-12727.6	0.995314
Protocatechuic acid	0.027	0.045	0.009	0.171	99.1-100.9	0.57	90.0-99.7	y=137.052x+1154.01	0.996650
<i>trans</i> -2-hydroxy cinnamic acid	0.063	0.105	0.021	0.252	98.1-99.9	1.27	92.1-100.8	y=417.594x-5112.34	0.998600
Gallic acid	0.048	0.080	0.016	0.192	98.6-100.8	0.49	95.4-99.7	y=721.654x+19597	0.997972

<b>Compound</b>	<b>LOD (mg 100 mL<sup>-1</sup>)</b>	<b>LOQ (mg 100 mL<sup>-1</sup>)</b>	<b>CV%<sup>a</sup></b>	<b>CV%<sup>b</sup></b>	<b>Recovery (%)<sup>b</sup></b>	<b>Stability CV%<sup>c</sup></b>	<b>Accuracy (%)<sup>d</sup></b>	<b>Calibration equations</b>	<b>r<sup>2</sup></b>
Myricetin	0.015	0.025	0.005	0.160	94.5-101.6	1.22	98.1-100.5	y=4.39568x-73.9242	0.994971
Naringenin	0.009	0.015	0.003	0.066	96.1-99.6	0.62	96.1-100.2	y=764.46x-3158.63	0.996254
Caffeic acid	0.054	0.090	0.018	0.216	89.9-99.1	1.03	98.1-100.2	y=133.554x+3121.08	0.993104
Pyrogallol	0.069	0.115	0.023	0.276	99.7-100.2	0.62	90.8-98.1	y=16.6558x-1173.34	0.990920
Luteolin	0.006	0.010	0.002	0.064	95.4-98.7	0.99	99.2-100.5	y=606.354x-17970.6	0.997617
Kaempferol	0.006	0.010	0.002	0.084	94.1-96.9	0.45	95.7-100.1	y=82.2591x-3446.02	0.990922

<sup>a</sup> Intra-day repeatability.

<sup>b</sup> Inter-day reproducibility and recovery from once a day of three consecutive days.

<sup>c</sup> Stability were measured by standard solutions over three consecutive days.

<sup>d</sup> Accuracy represents the ratio of the measured concentration to the theoretical concentration from medium concentration value of the calibration range.