

# Identification of Chemical Constituents in *Blumea balsamifera* Using UPLC–Q–Orbitrap HRMS and Evaluation of Their Antioxidant Activities

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and Wei Dai <sup>2,\*</sup>

**Figure S1.** MS<sup>2</sup> fragmentation spectra (CID) of  $\alpha,\alpha$ -trehalose

**Figure S2.** MS<sup>2</sup> fragmentation spectra (CID) of D-(–)-fructose

**Figure S3.** MS<sup>2</sup> fragmentation spectra (CID) of gentisic acid 5-O- $\beta$ -glucoside

**Figure S4.** MS<sup>2</sup> fragmentation spectra (CID) of caffeic acid

**Figure S5.** MS<sup>2</sup> fragmentation spectra (CID) of tuberonic acid glucoside

**Figure S6.** MS<sup>2</sup> fragmentation spectra (CID) of hemiphloin

**Figure S7.** MS<sup>2</sup> fragmentation spectra (CID) of taxifolin

**Figure S8.** MS<sup>2</sup> fragmentation spectra (CID) of rutin

**Figure S9.** MS<sup>2</sup> fragmentation spectra (CID) of quercetin-3 $\beta$ -D-glucoside

**Figure S10.** MS<sup>2</sup> fragmentation spectra (CID) of quercetin

**Figure S11.** MS<sup>2</sup> fragmentation spectra (CID) of quercetin-3-Arabinoside

**Figure S12.** MS<sup>2</sup> fragmentation spectra (CID) of cynaroside

**Figure S13.** MS<sup>2</sup> fragmentation spectra (CID) of 1,3-Dicaffeoylquinic acid

**Figure S14.** MS<sup>2</sup> fragmentation spectra (CID) of chlorogenic acid

**Figure S15.** MS<sup>2</sup> fragmentation spectra (CID) of isorhamnetin-3-O-glucoside

**Figure S16.** MS<sup>2</sup> fragmentation spectra (CID) of 4-oxo-5-phenylpentanoic acid

**Figure S17.** MS<sup>2</sup> fragmentation spectra (CID) of eriodictyol

**Figure S18.** MS<sup>2</sup> fragmentation spectra (CID) of padmatin

**Figure S19.** MS<sup>2</sup> fragmentation spectra (CID) of isorhamnetin

**Figure S20.** MS<sup>2</sup> fragmentation spectra (CID) of naringenin

**Figure S21.** MS<sup>2</sup> fragmentation spectra (CID) of 7-O-Methylaromadendrin

**Figure S22.** MS<sup>2</sup> fragmentation spectra (CID) of aurantio-obtusin

**Figure S23.** MS<sup>2</sup> fragmentation spectra (CID) of fraxetin

**Figure S24.** MS<sup>2</sup> fragmentation spectra (CID) of hematoxylin

**Figure S25.** MS<sup>2</sup> fragmentation spectra (CID) of sakuranetin

**Figure S26.** MS<sup>2</sup> fragmentation spectra (CID) of aurantiamide acetate

**Figure S27.** MS<sup>2</sup> fragmentation spectra (CID) of cryptotanshinone

**Figure S28.** MS<sup>2</sup> fragmentation spectra (CID) of nootkatone

**Figure S29.** MS<sup>2</sup> fragmentation spectra (CID) of N-Phenyl-1-naphthylamine

**Figure S30.** MS<sup>2</sup> fragmentation spectra (CID) of tanshinone IIA

**Figure S31.** MS<sup>2</sup> fragmentation spectra (CID) of citroflex A-4

**Figure S32.** TICs of *Blumea balsamifera* ( L. ) DC. in negative ion mode

**Figure S33.** TICs of *Blumea balsamifera* ( L. ) DC. in positive ion mode

ANX-100%JC-Nd #952 RT: 0.86 AV: 1 NL: 2.55E5  
F: FTMS -p ESI d Full ms2 341.1084@hcd40.00 [50.0000-368.6956]

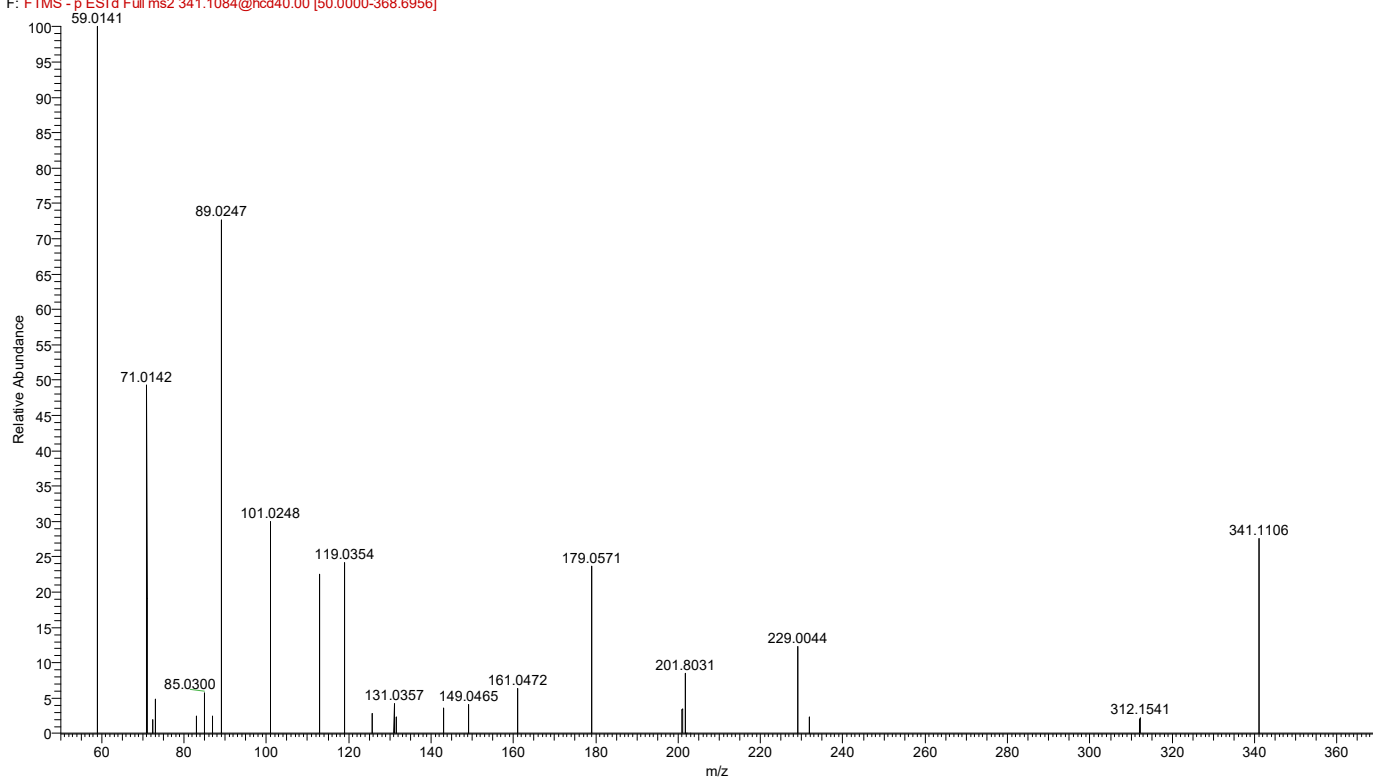


Figure S1. MS<sup>2</sup> fragmentation spectra (CID) of  $\alpha,\alpha$ -trehalose

ANX-100%JC-Nd #941 RT: 0.85 AV: 1 NL: 5.14E5  
F: FTMS -p ESI d Full ms2 179.0558@hcd40.00 [40.6804-203.4019]

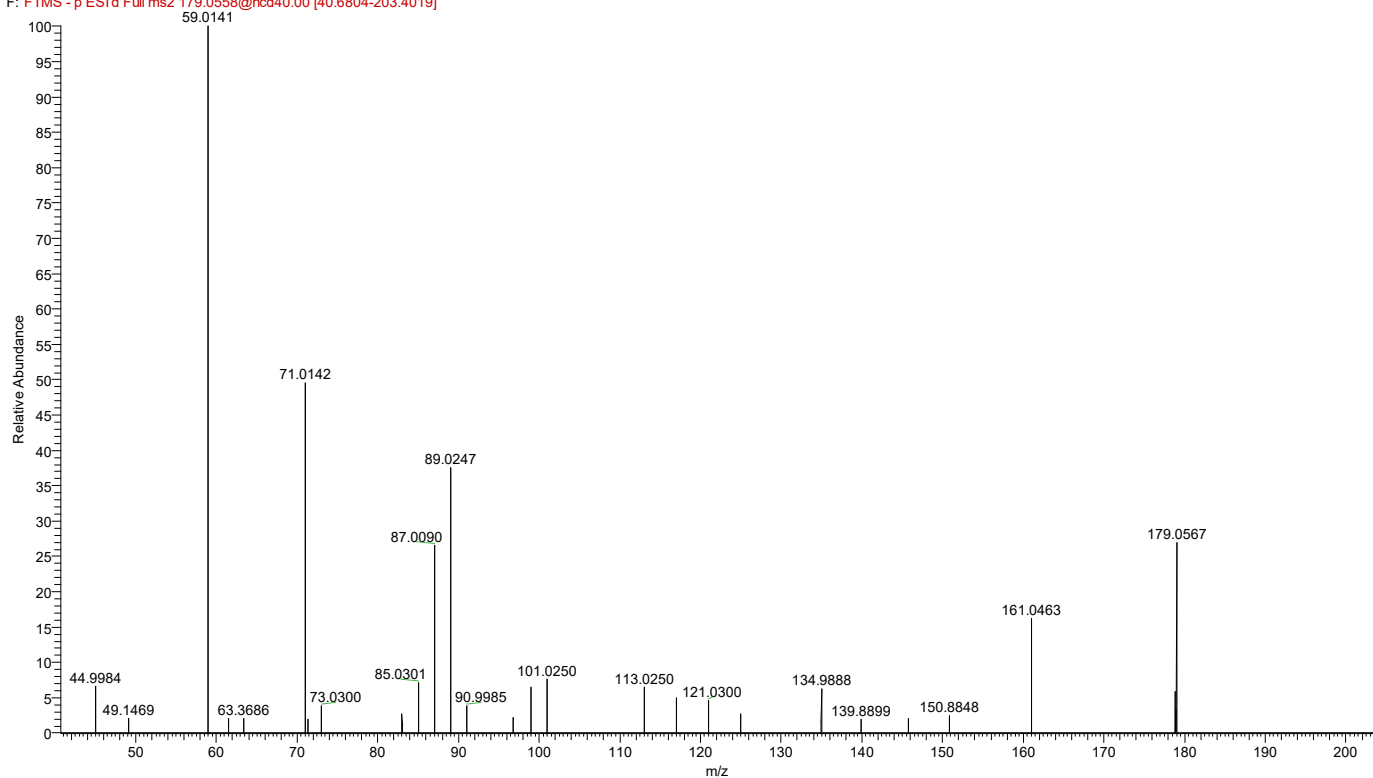
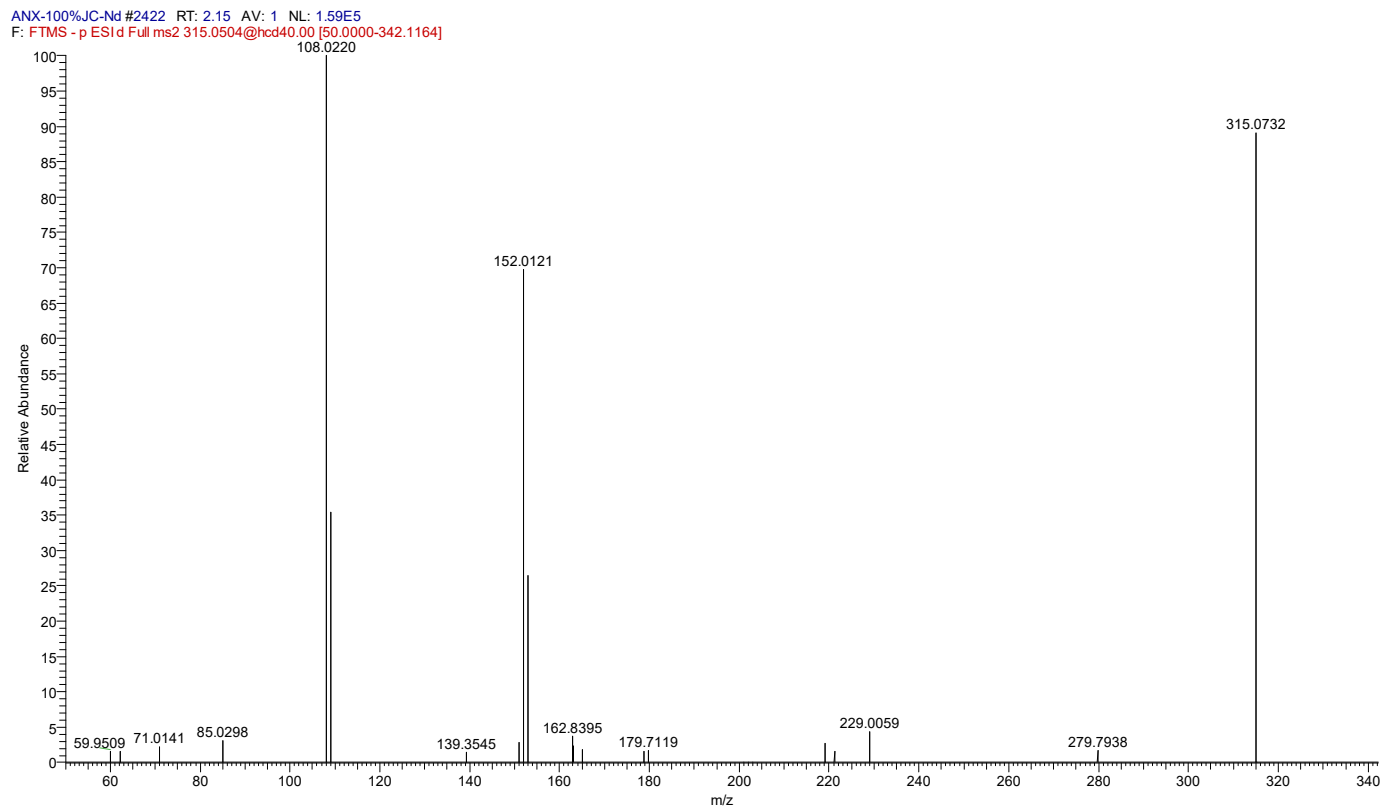
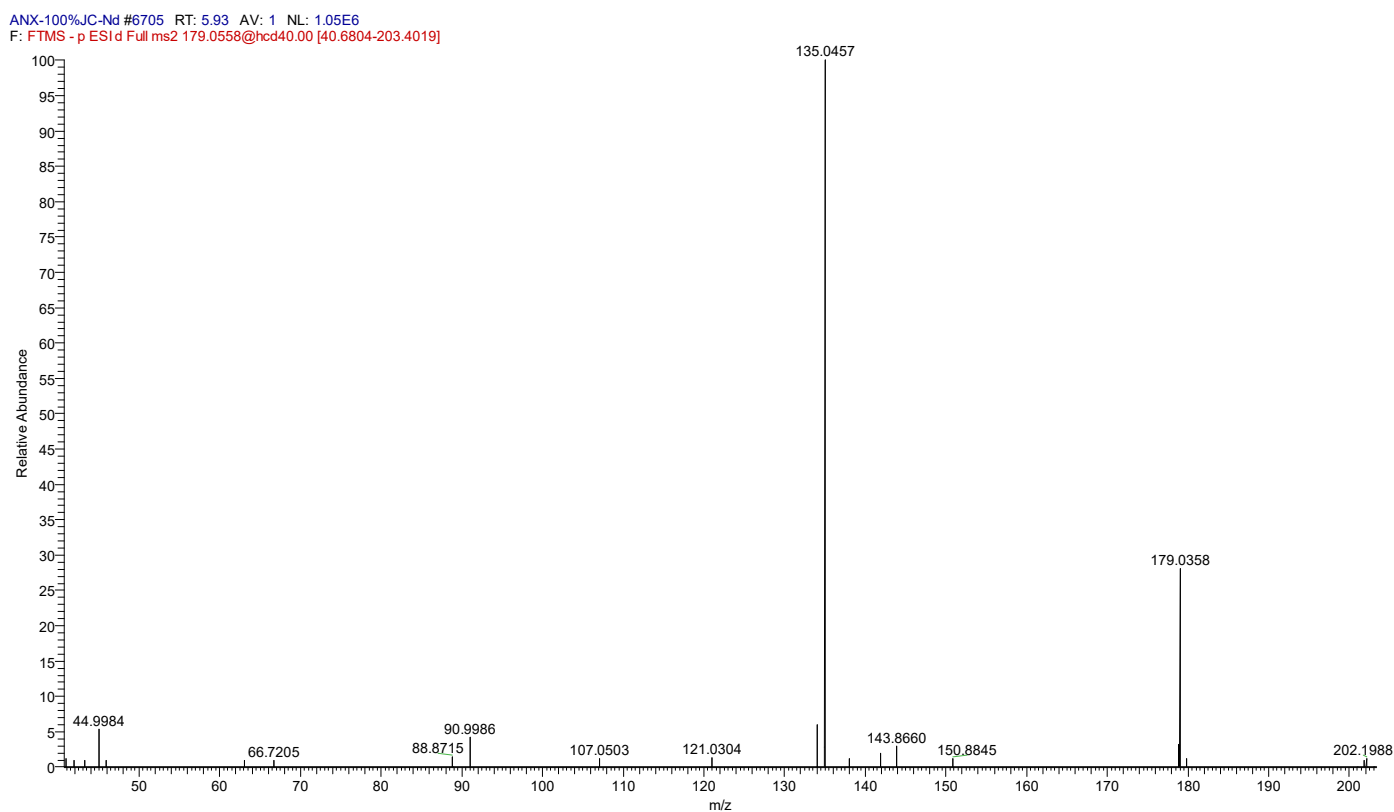


Figure S2. MS<sup>2</sup> fragmentation spectra (CID) of D-(-)-fructose

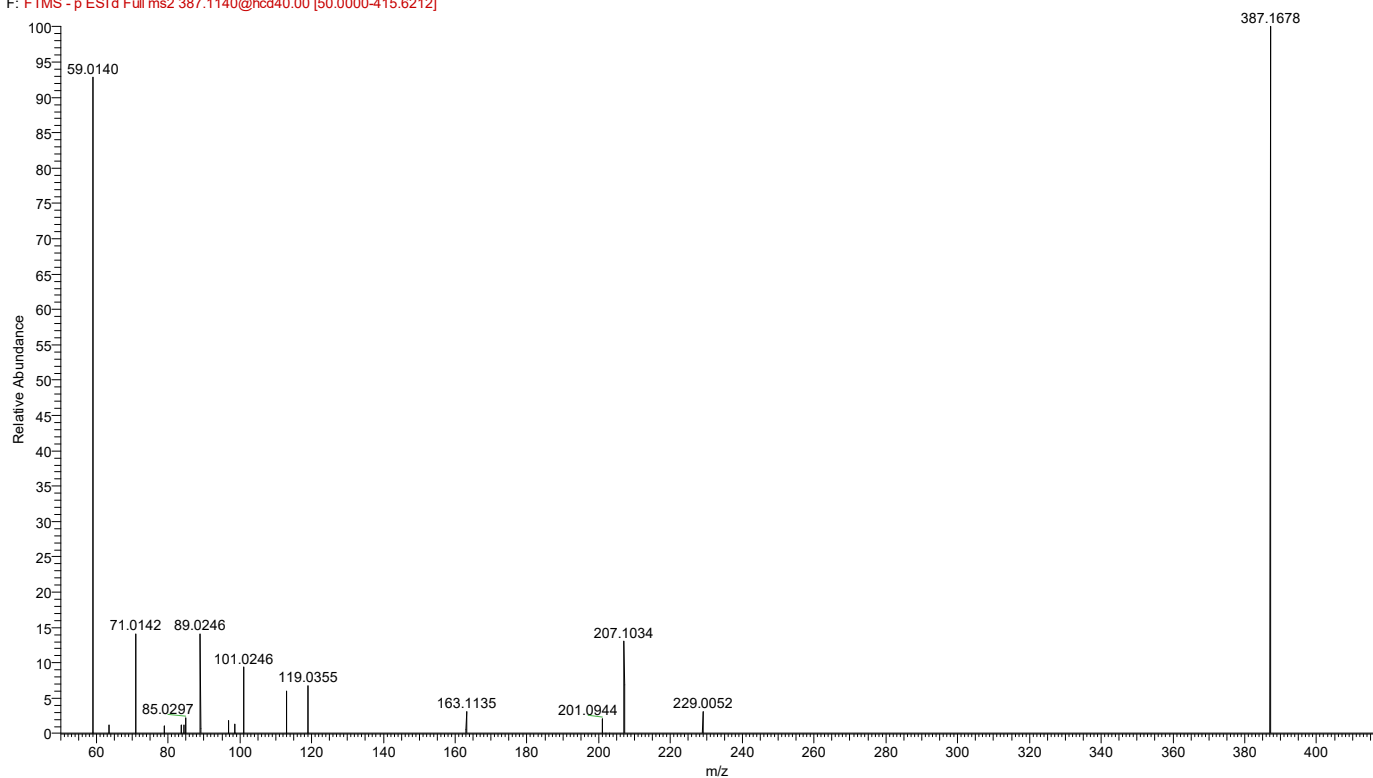


**Figure S3.** MS<sup>2</sup> fragmentation spectra (CID) of gentisic acid 5-O- $\beta$ -glucoside



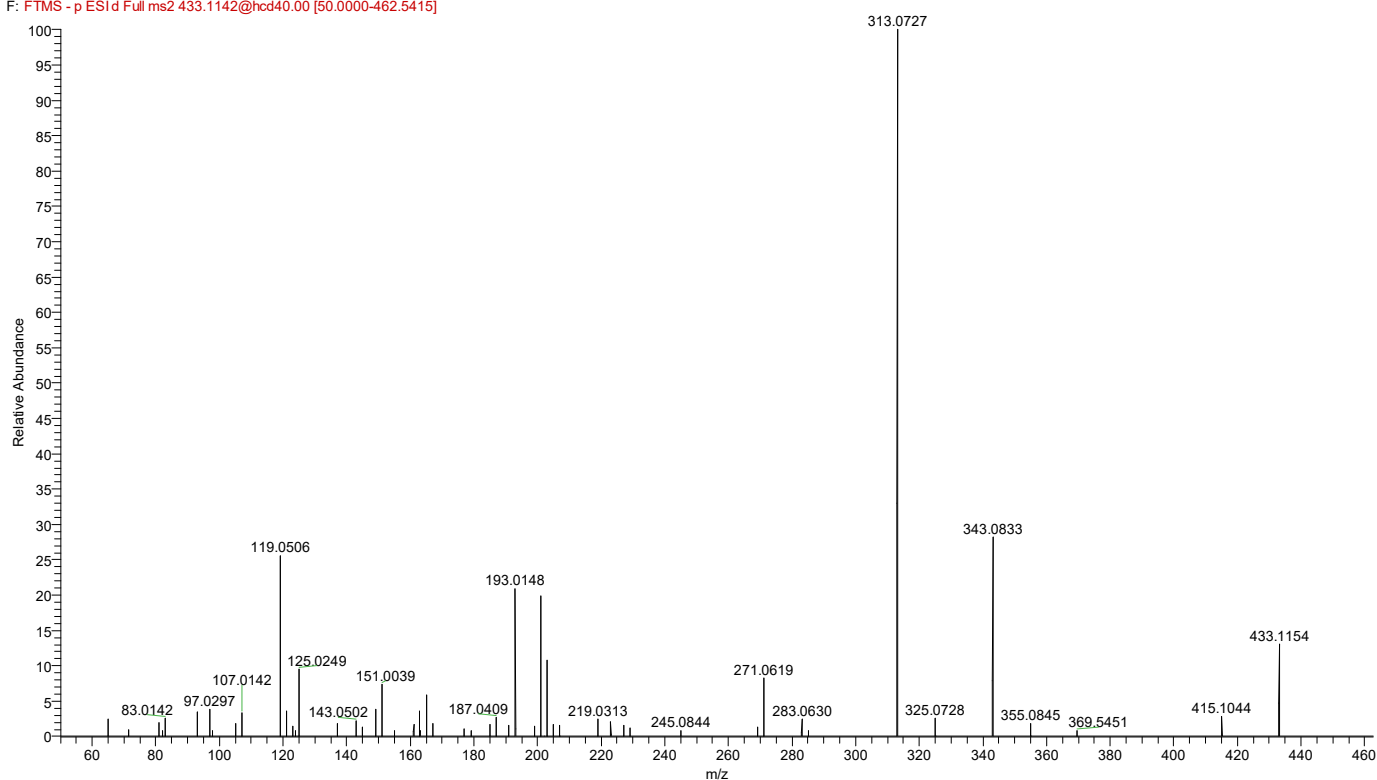
**Figure S4.** MS<sup>2</sup> fragmentation spectra (CID) of caffeic acid

ANX-100%JC-Nd #8187 RT: 7.23 AV: 1 NL: 2.21E5  
F: FTMS -p ESI d Full ms2 387.1140@hcd40.00 [50.0000-415.6212]



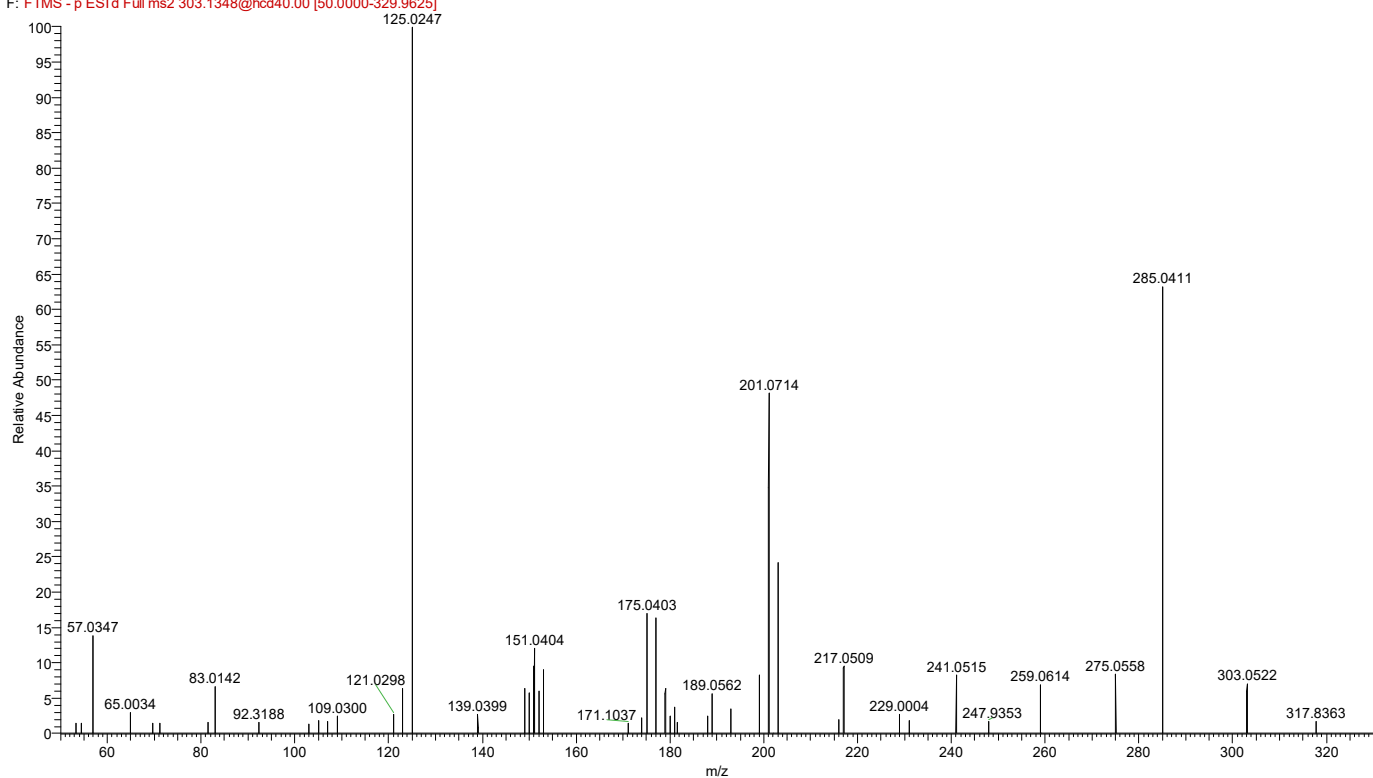
**Figure S5.** MS<sup>2</sup> fragmentation spectra (CID) of tuberonic acid glucoside

ANX-100%JC-Nd #11533 RT: 10.18 AV: 1 NL: 3.45E6  
F: FTMS -p ESI d Full ms2 433.1142@hcd40.00 [50.0000-462.5415]



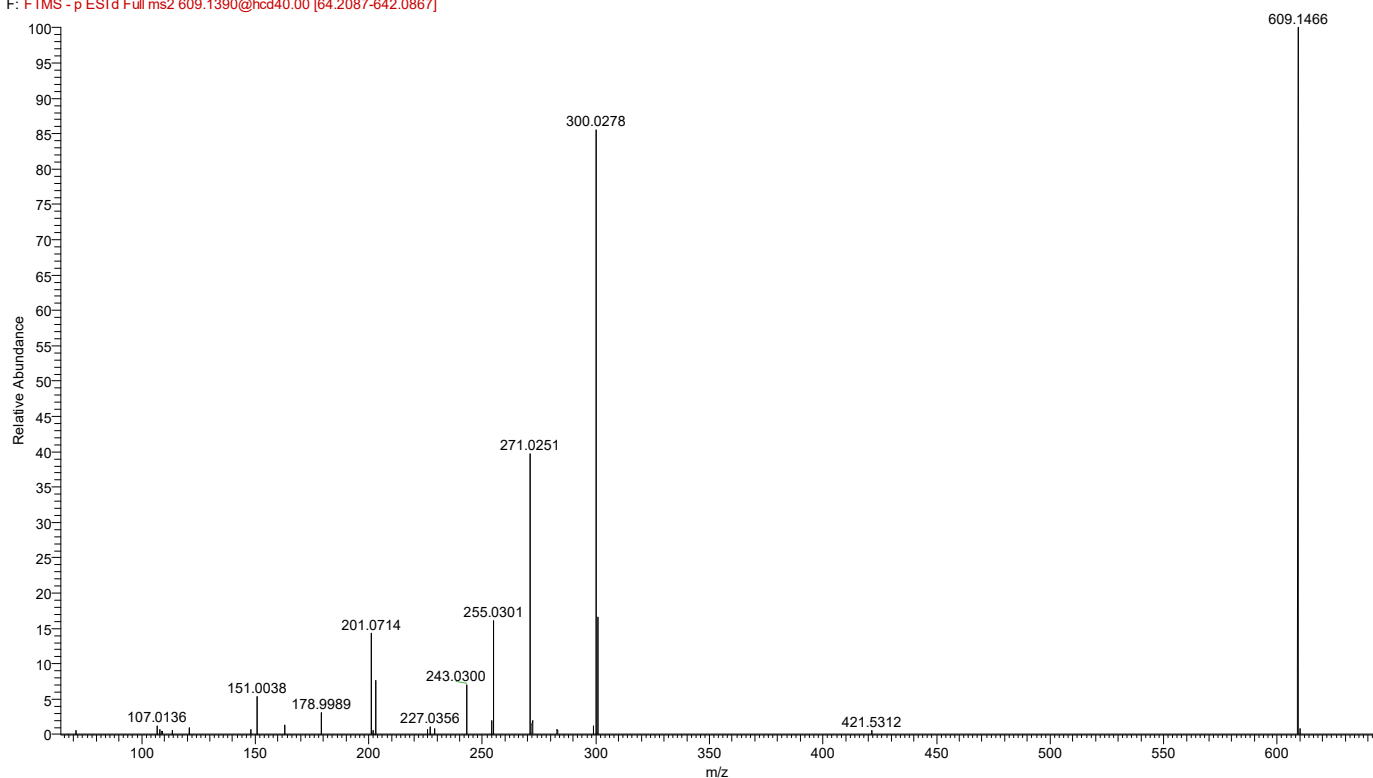
**Figure S6.** MS<sup>2</sup> fragmentation spectra (CID) of hemiphloin

ANX-100%JC-Nd #11762 RT: 10.38 AV: 1 NL: 1.66E5  
F: FTMS -p ESI d Full ms2 303.1348@hcd40.00 [50.0000-329.9625]



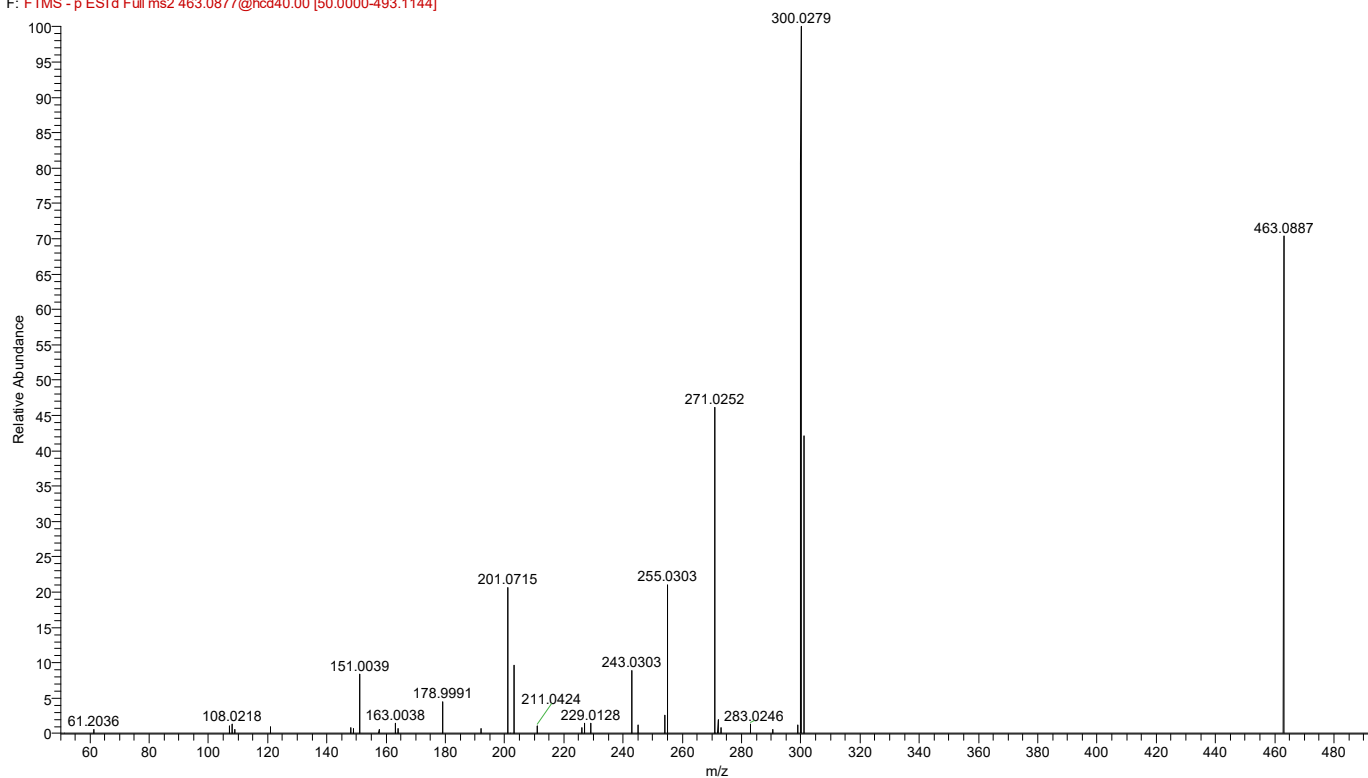
**Figure S7.** MS<sup>2</sup> fragmentation spectra (CID) of taxifolin

ANX-100%JC-Nd #11827 RT: 10.44 AV: 1 NL: 1.12E6  
F: FTMS -p ESI d Full ms2 609.1390@hcd40.00 [64.2087-642.0867]



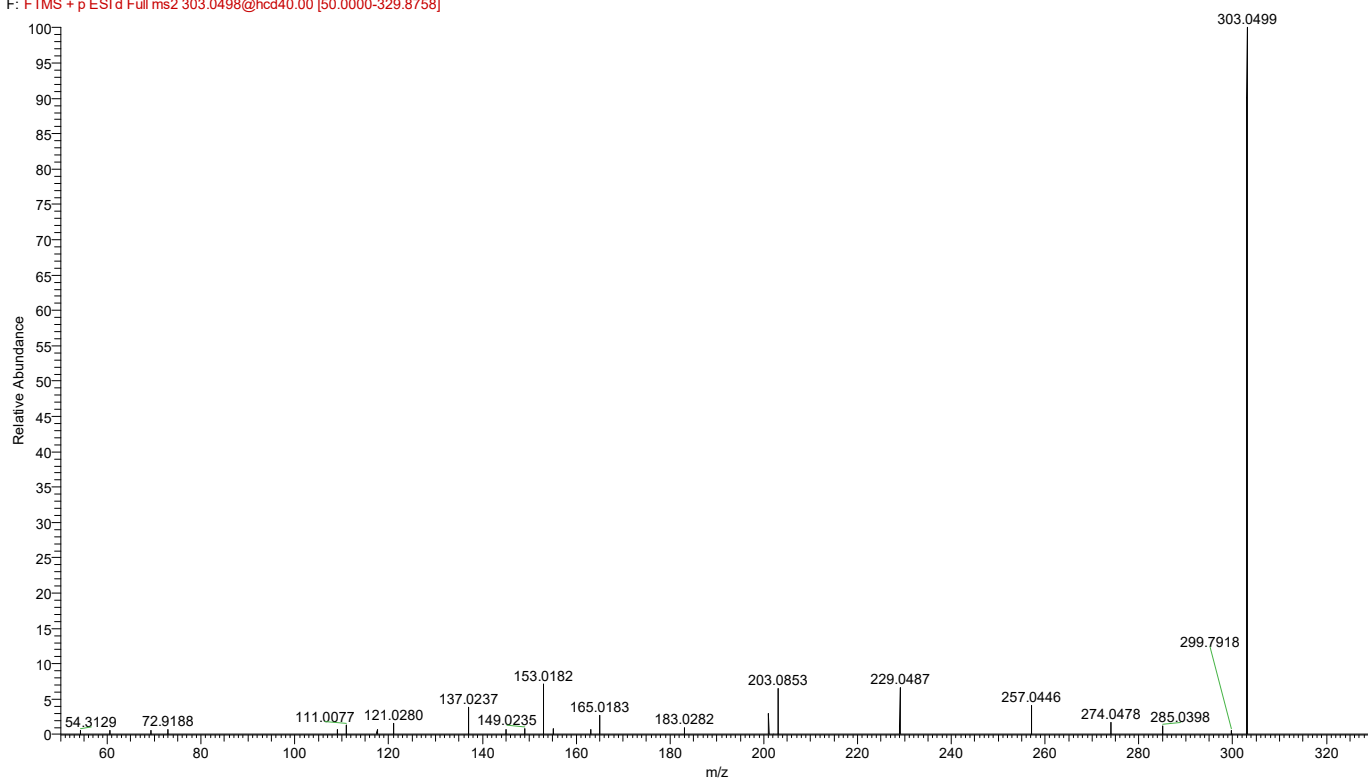
**Figure S8.** MS<sup>2</sup> fragmentation spectra (CID) of rutin

ANX-100%JC-Nd #12480 RT: 11.02 AV: 1 NL: 1.73E6  
F: FTMS - p ESI d Full ms2 463.0877@hcd40.00 [50.0000-493.1144]



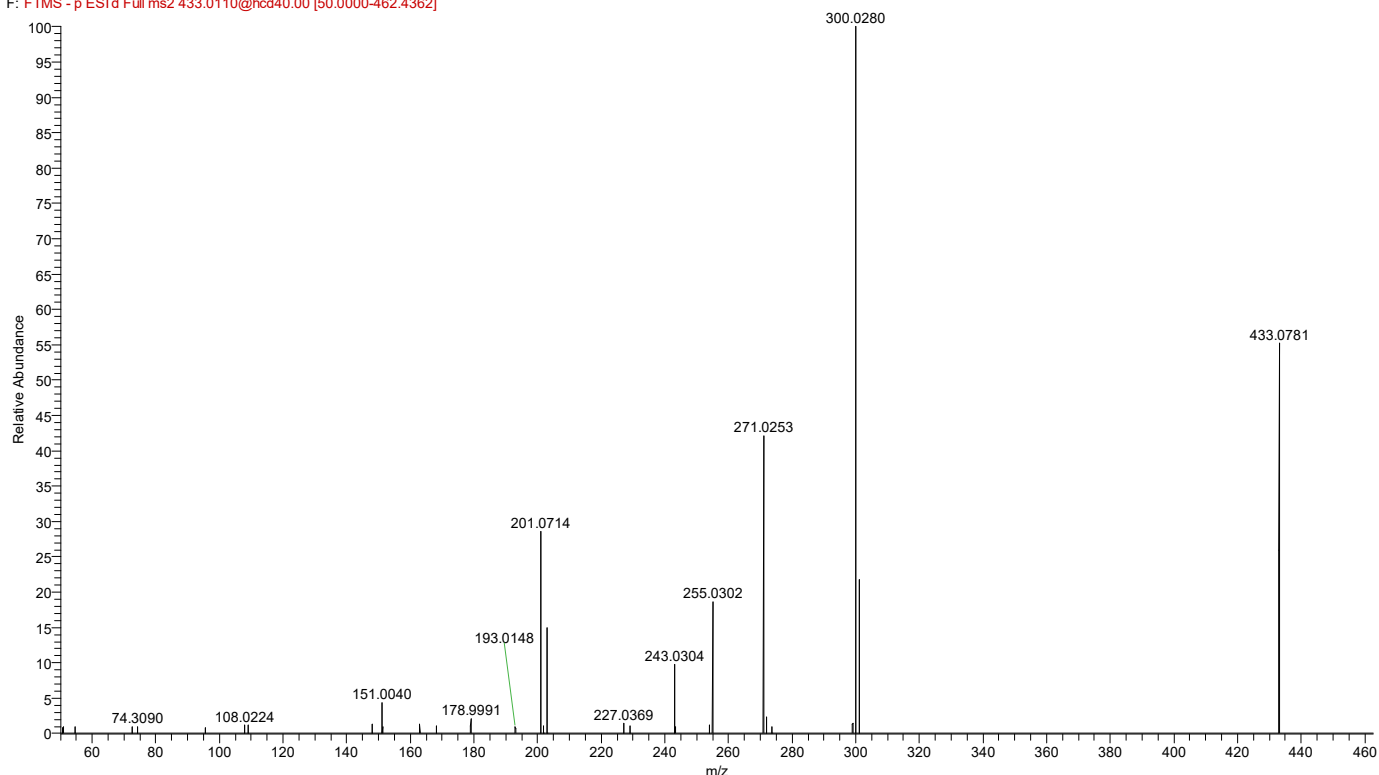
**Figure S9.** MS<sup>2</sup> fragmentation spectra (CID) of quercetin-3 $\beta$ -D-glucoside

ANX-100%JC-Pd #12781 RT: 11.14 AV: 1 NL: 6.41E5  
F: FTMS + p ESI d Full ms2 303.0498@hcd40.00 [50.0000-329.8758]



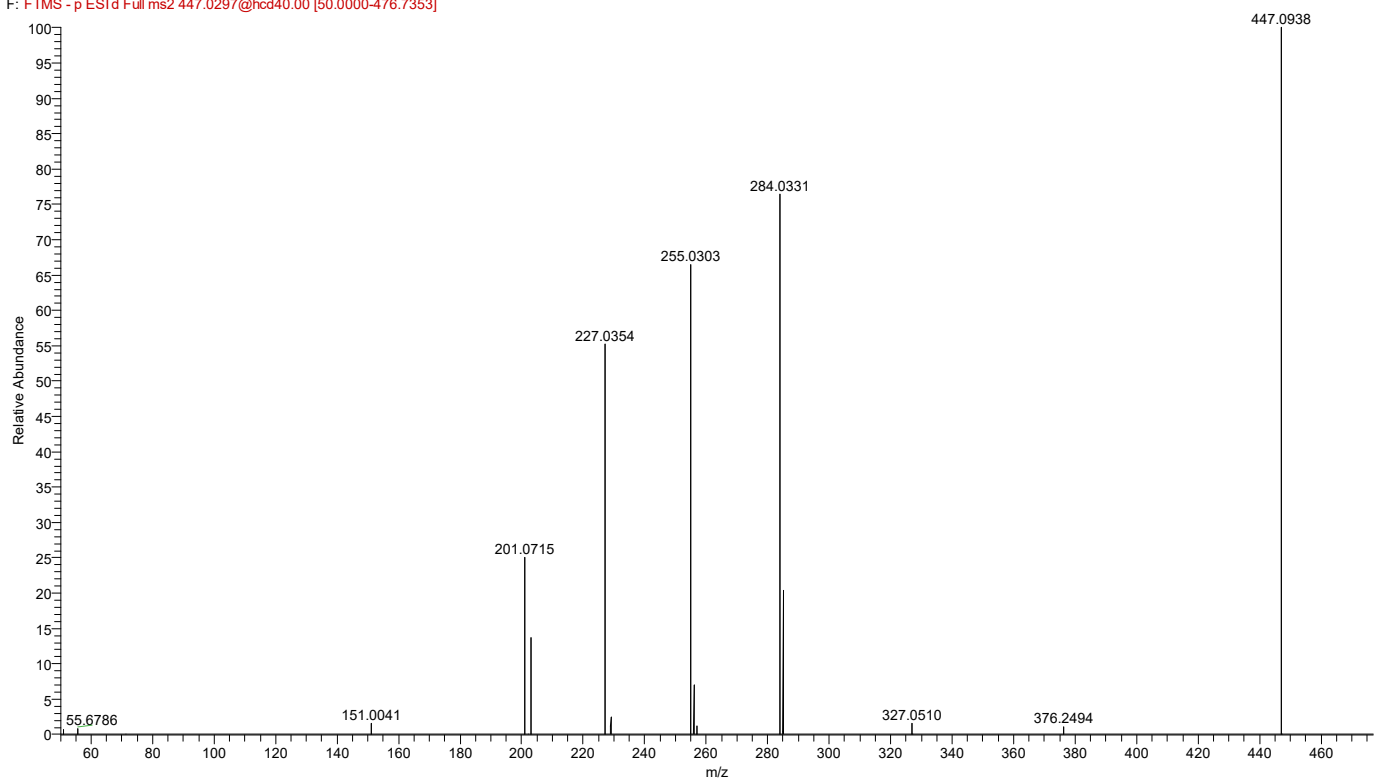
**Figure S10.** MS<sup>2</sup> fragmentation spectra (CID) of quercetin

ANX-100%JC-Nd #13649 RT: 12.05 AV: 1 NL: 2.77E5  
F: FTMS -p ES1d Full ms2 433.0110@hcd40.00 [50.0000-462.4362]



**Figure S11.** MS<sup>2</sup> fragmentation spectra (CID) of quercetin-3-Arabinoside

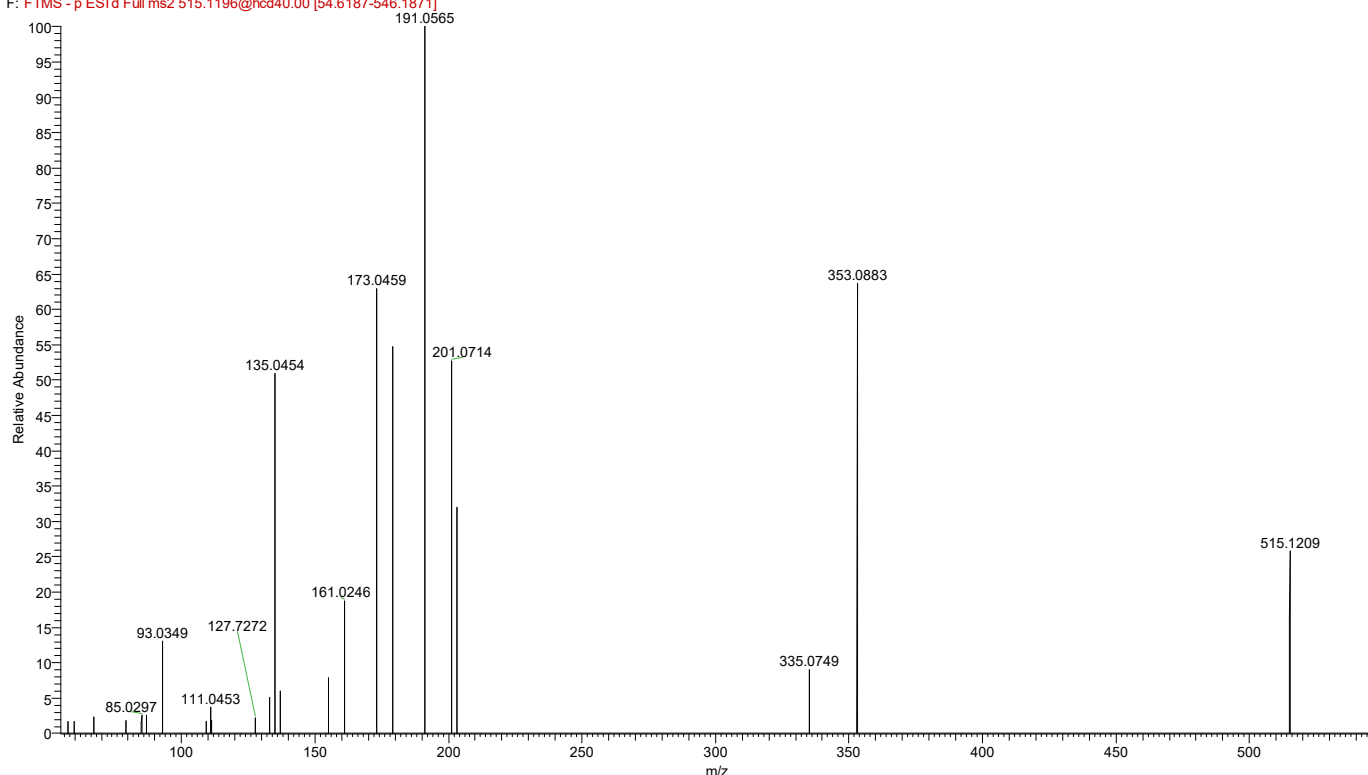
ANX-100%JC-Nd #13684 RT: 12.08 AV: 1 NL: 4.08E5  
F: FTMS -p ES1d Full ms2 447.0297@hcd40.00 [50.0000-476.7353]



**Figure S12.** MS<sup>2</sup> fragmentation spectra (CID) of cynaroside

ANX-100%JC-Nd #14166 RT: 12.50 AV: 1 NL: 1.39E5

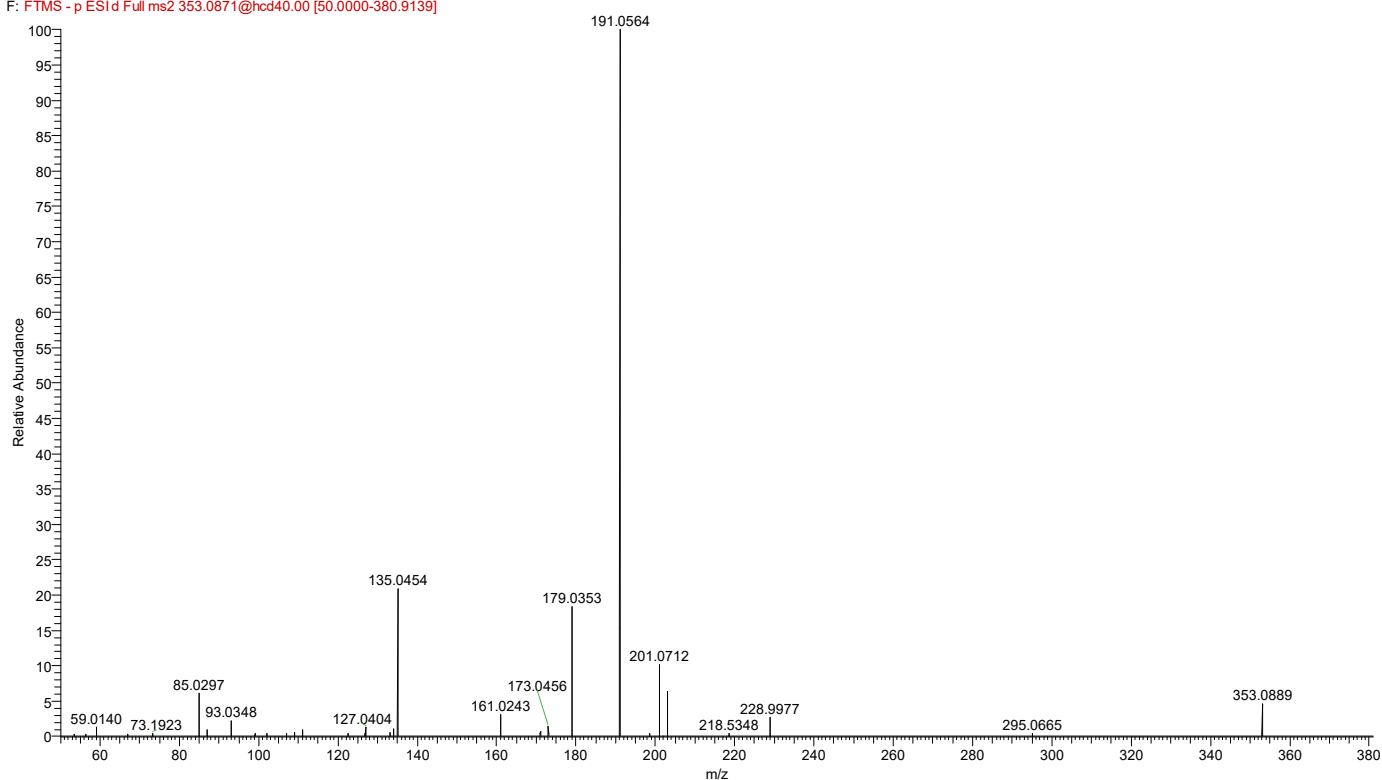
F: FTMS -p ESId Full ms2 515.1196@hcd40.00 [54.6187-546.1871]



**Figure S13.** MS<sup>2</sup> fragmentation spectra (CID) of 1,3-Dicaffeoylquinic acid

ANX-100%JC-Nd #14371 RT: 12.68 AV: 1 NL: 6.78E5

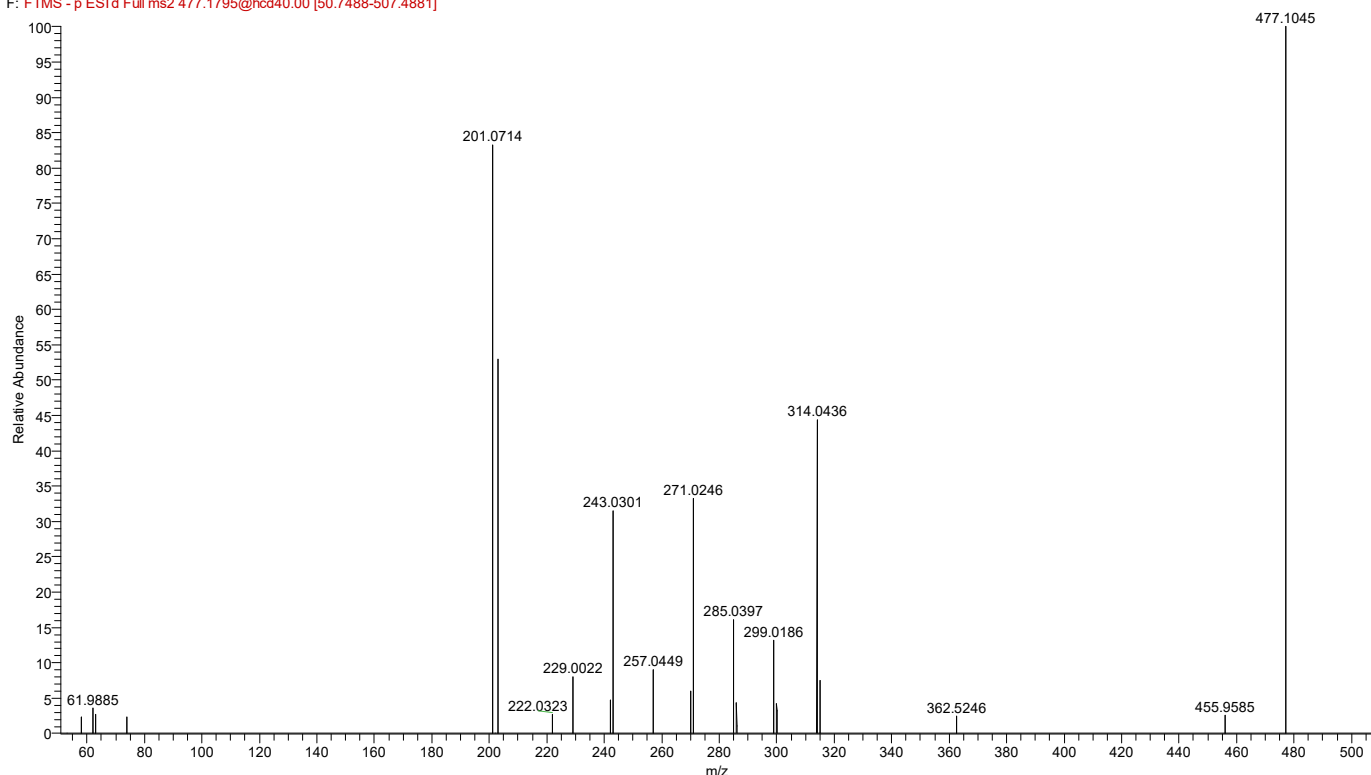
F: FTMS -p ESId Full ms2 353.0871@hcd40.00 [50.0000-380.9139]



**Figure S14.** MS<sup>2</sup> fragmentation spectra (CID) of chlorogenic acid

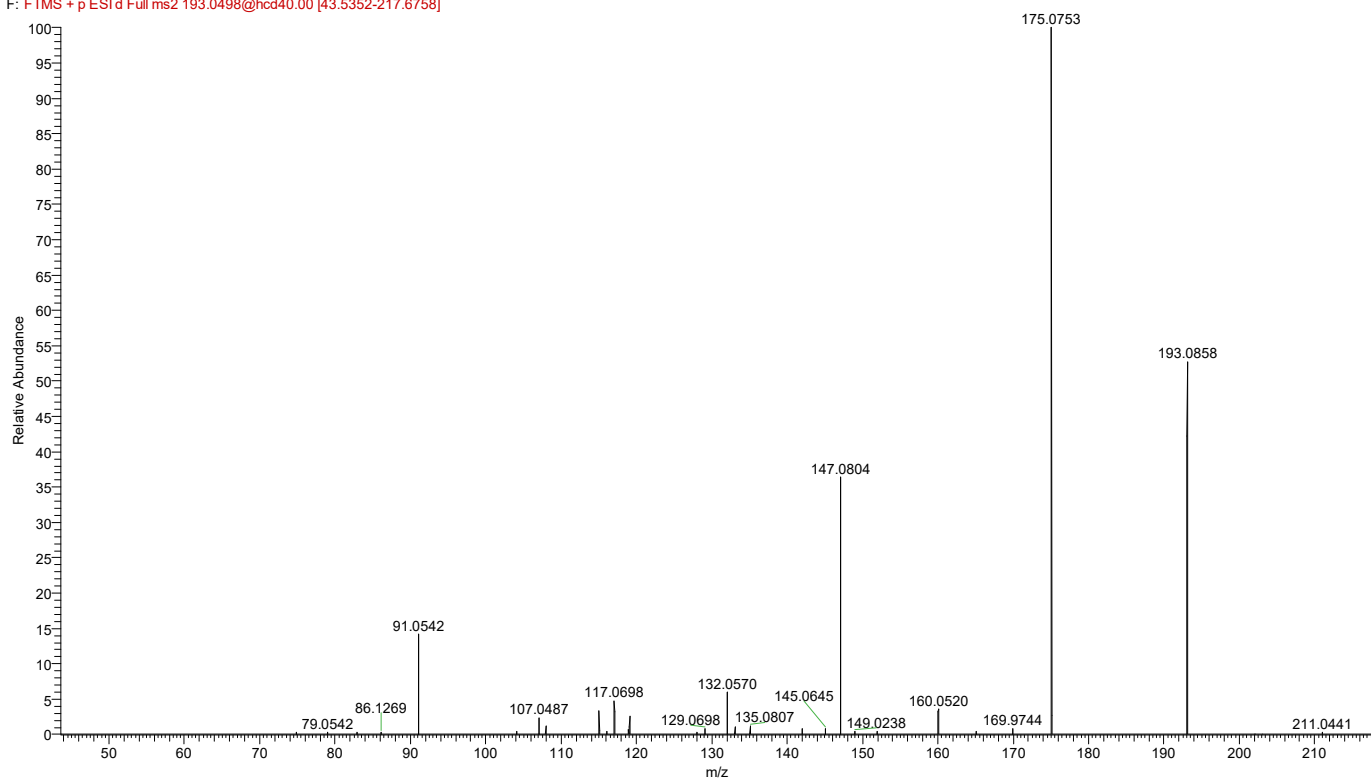


ANX-100%JC-Nd #14806 RT: 13.07 AV: 1 NL: 1.01E5  
F: FTMS -p ESI d Full ms2 477.1795@hcd40.00 [50.7488-507.4881]



**Figure S15.** MS<sup>2</sup> fragmentation spectra (CID) of isorhamnetin-3-O-glucoside

ANX-100%JC-Pd #15453 RT: 13.47 AV: 1 NL: 1.29E6  
F: FTMS +p ESI d Full ms2 193.0498@hcd40.00 [43.5352-217.6758]



**Figure S16.** MS<sup>2</sup> fragmentation spectra (CID) of 4-oxo-5-phenylpentanoic acid

ANX-100%JC-Nd #18449 RT: 16.28 AV: 1 NL: 4.94E6  
F: FTMS -p ESId Full ms2 287.0438@hcd40.00 [50.0000-313.5497]

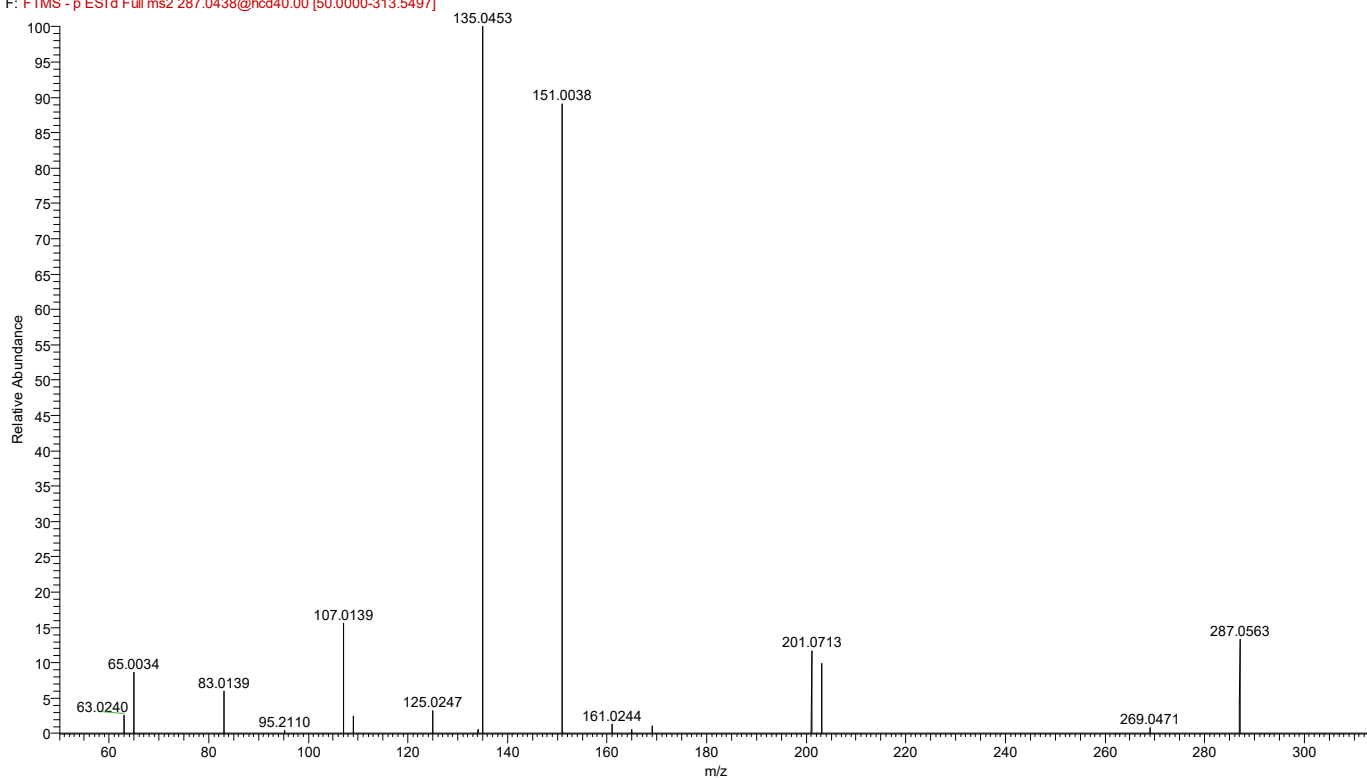


Figure S17. MS<sup>2</sup> fragmentation spectra (CID) of eriodictyol

ANX-100%JC-Nd #20150 RT: 17.78 AV: 1 NL: 1.20E5  
F: FTMS -p ESId Full ms2 317.0050@hcd40.00 [50.0000-344.1101]

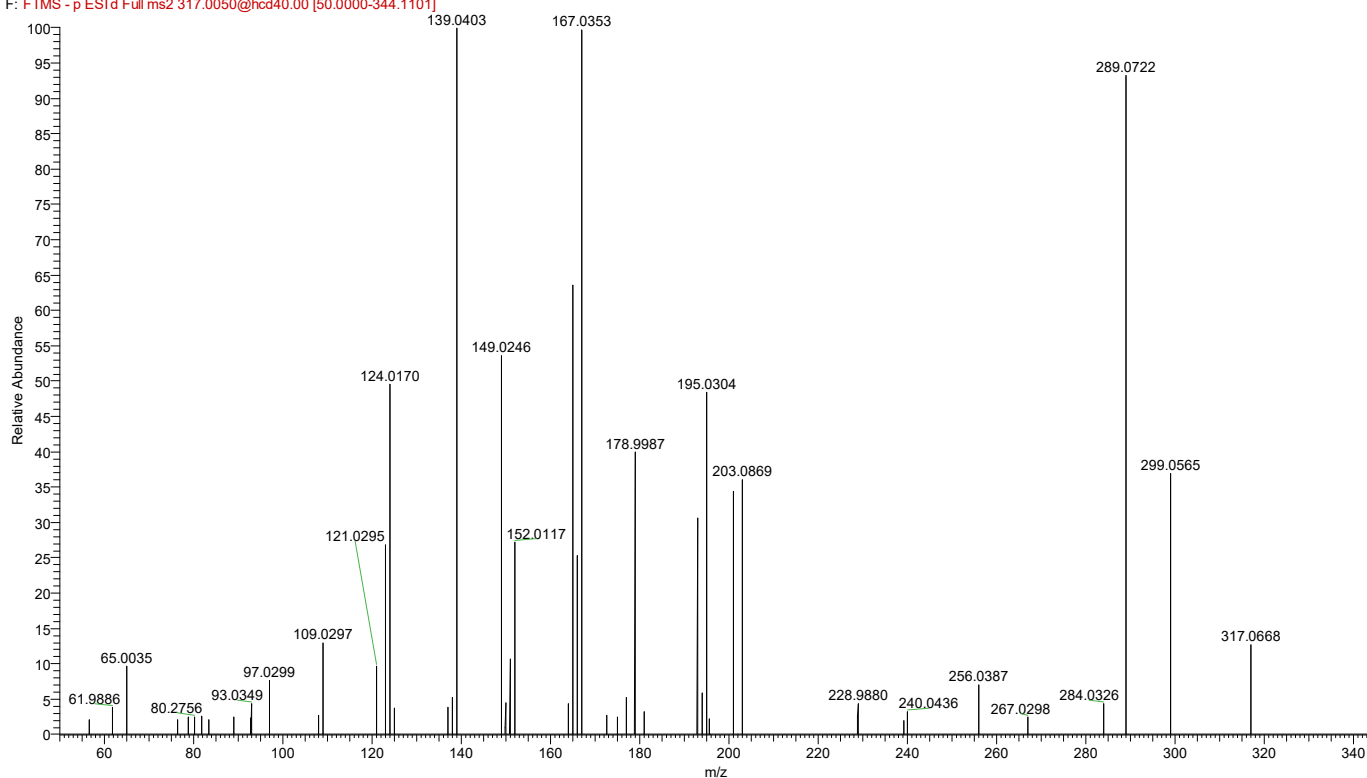
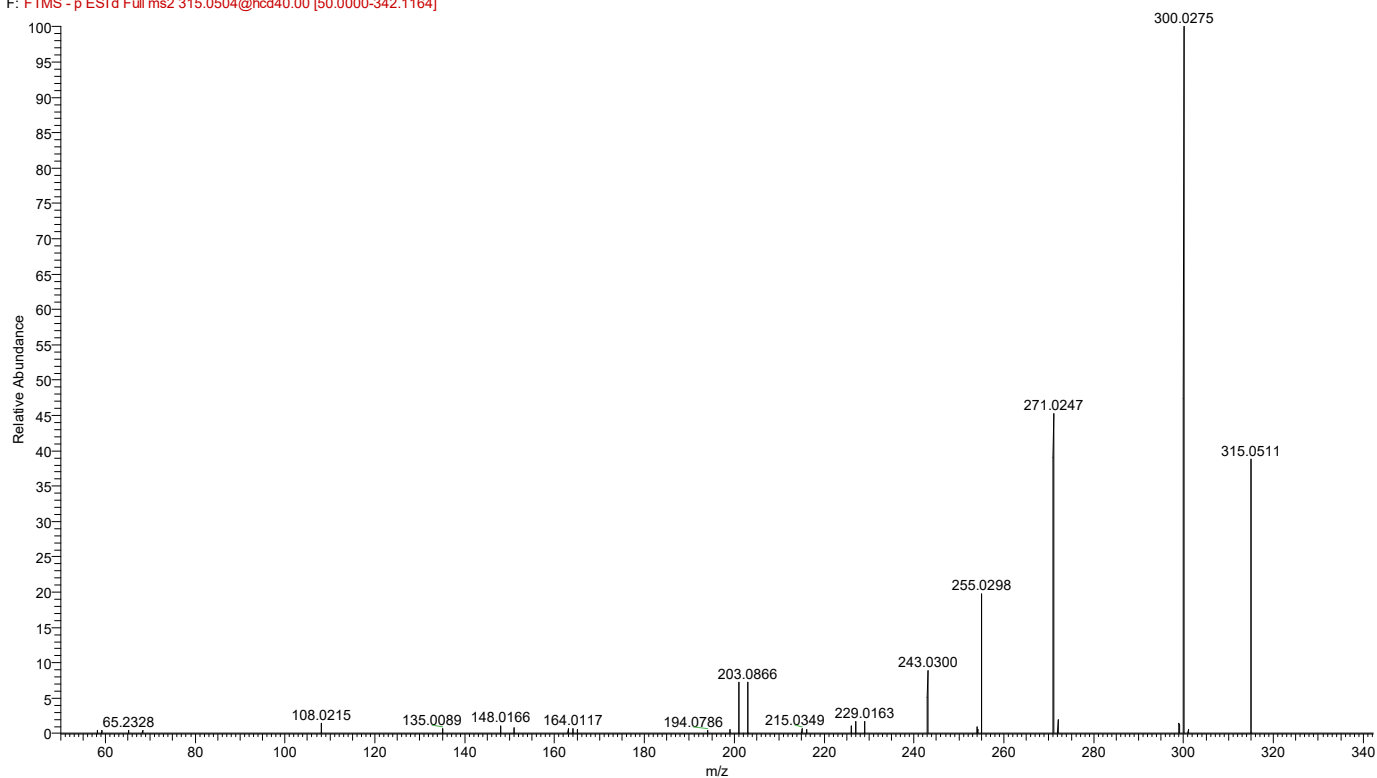


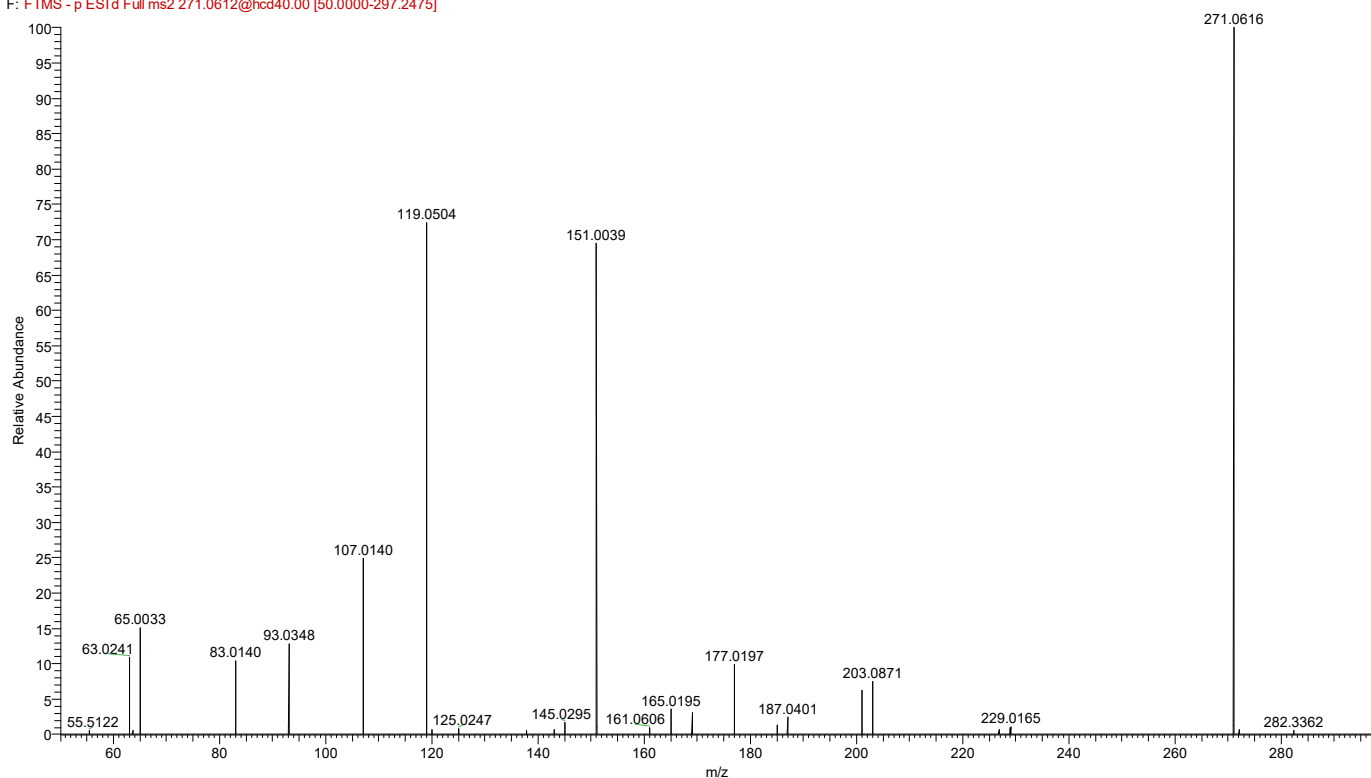
Figure S18. MS<sup>2</sup> fragmentation spectra (CID) of padmatin

ANX-100%JC-Nd #20340 RT: 17.95 AV: 1 NL: 8.66E5  
F: FTMS -p ESI d Full ms2 315.0504@hcd40.00 [50.0000-342.1164]



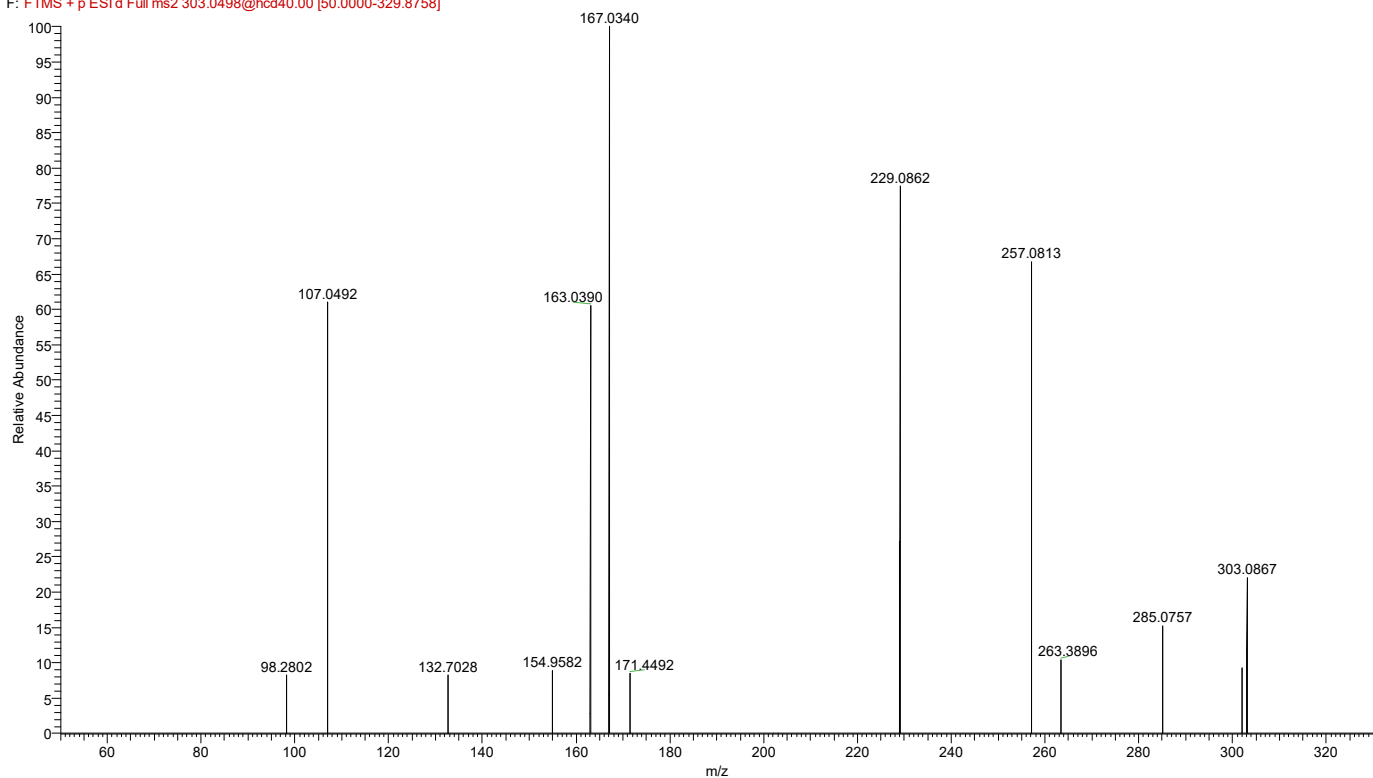
**Figure S19.** MS<sup>2</sup> fragmentation spectra (CID) of isorhamnetin

ANX-100%JC-Nd #20830 RT: 18.39 AV: 1 NL: 4.52E5  
F: FTMS -p ESI d Full ms2 271.0612@hcd40.00 [50.0000-297.2475]



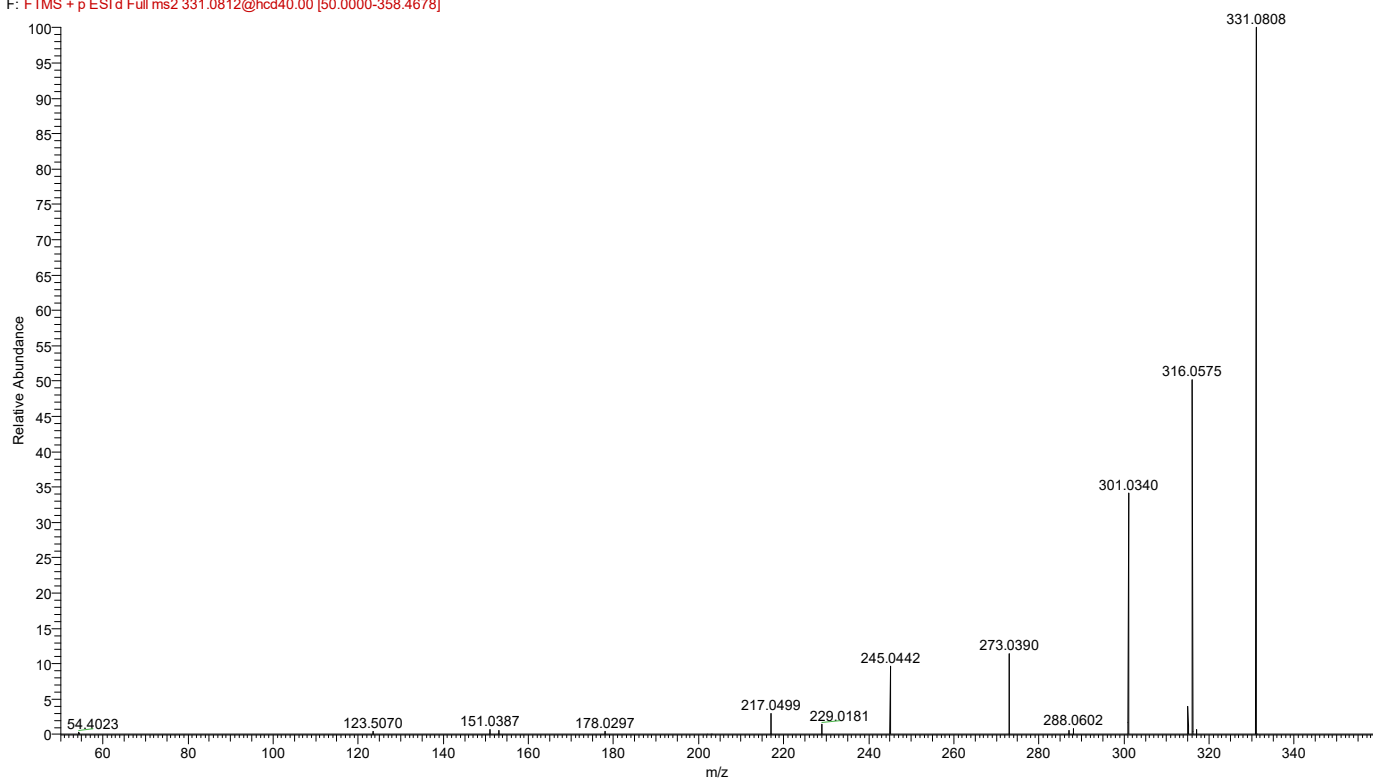
**Figure S20.** MS<sup>2</sup> fragmentation spectra (CID) of naringenin

ANX-100%JC-Pd #21939 RT: 19.12 AV: 1 NL: 1.19E5  
F: FTMS + p ESI d Full ms2 303.0498@hcd40.00 [50.0000-329.8758]



**Figure S21.** MS<sup>2</sup> fragmentation spectra (CID) of 7-O-Methylaromadendrin

ANX-100%JC-Pd #22293 RT: 19.43 AV: 1 NL: 2.59E6  
F: FTMS + p ESI d Full ms2 331.0812@hcd40.00 [50.0000-358.4678]



**Figure S22.** MS<sup>2</sup> fragmentation spectra (CID) of aurantio-obtusin

ANX-100%JC-Pd #22218 RT: 19.36 AV: 1 NL: 6.01E5  
F: FTMS + p ESI d Full ms2 209.0809@hcd40.00 [46.8055-234.0275]

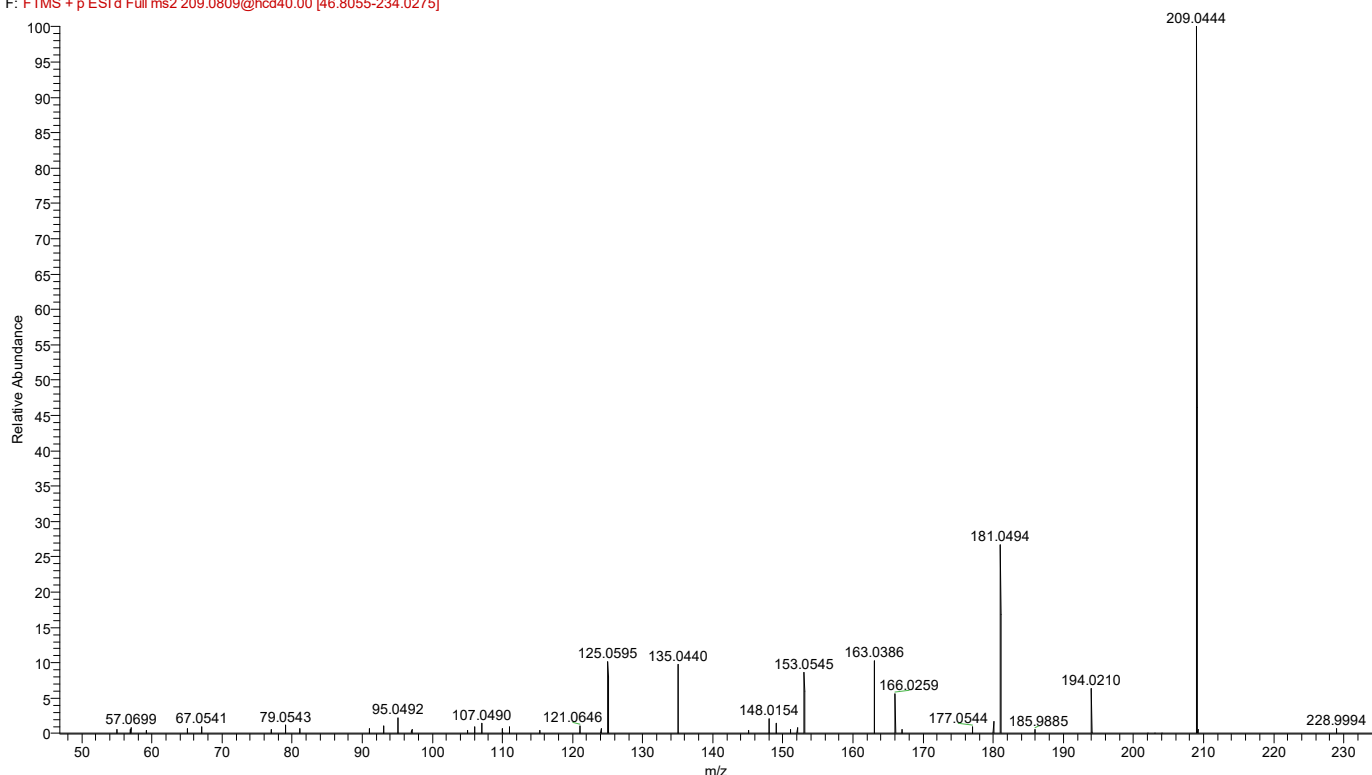


Figure S23. MS<sup>2</sup> fragmentation spectra (CID) of fraxetin

ANX-100%JC-Nd #22430 RT: 19.80 AV: 1 NL: 2.52E7  
F: FTMS - p ESI d Full ms2 301.0712@hcd40.00 [50.0000-327.8576]

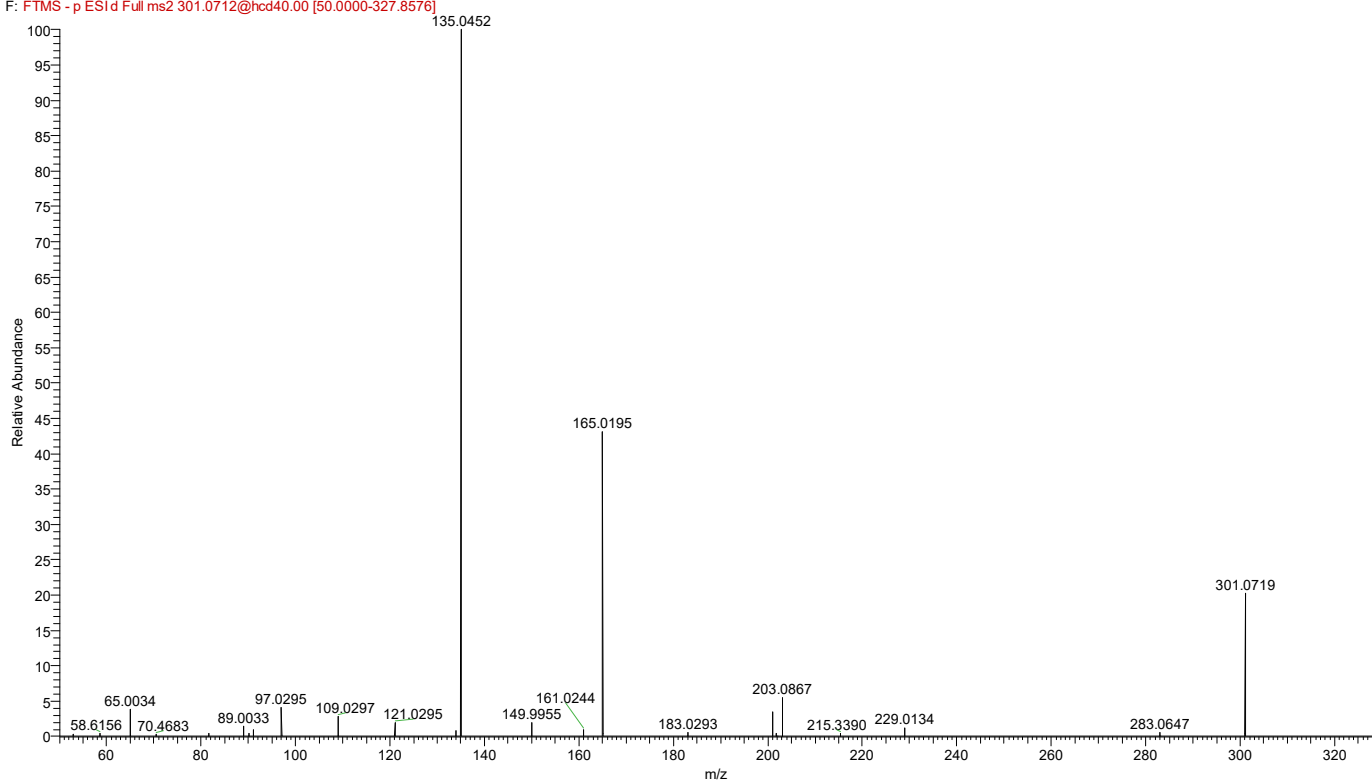
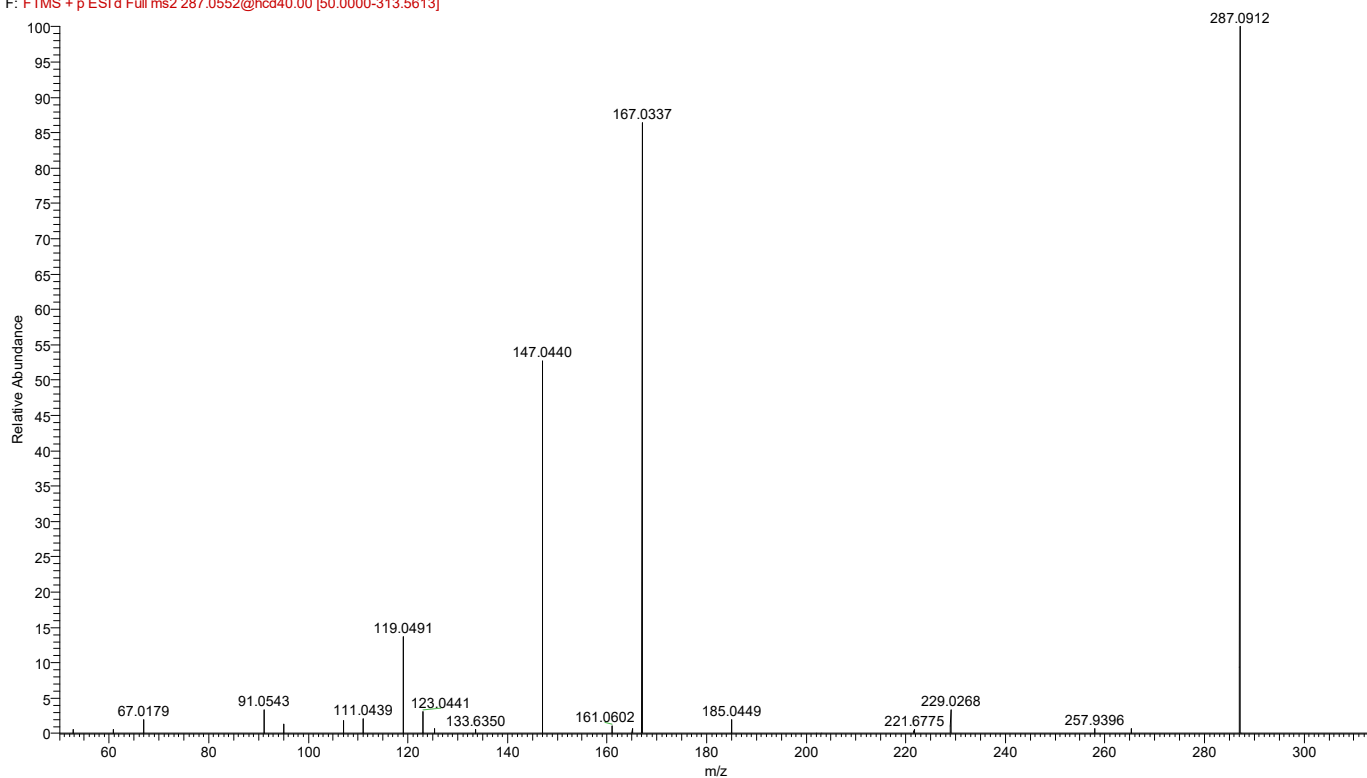


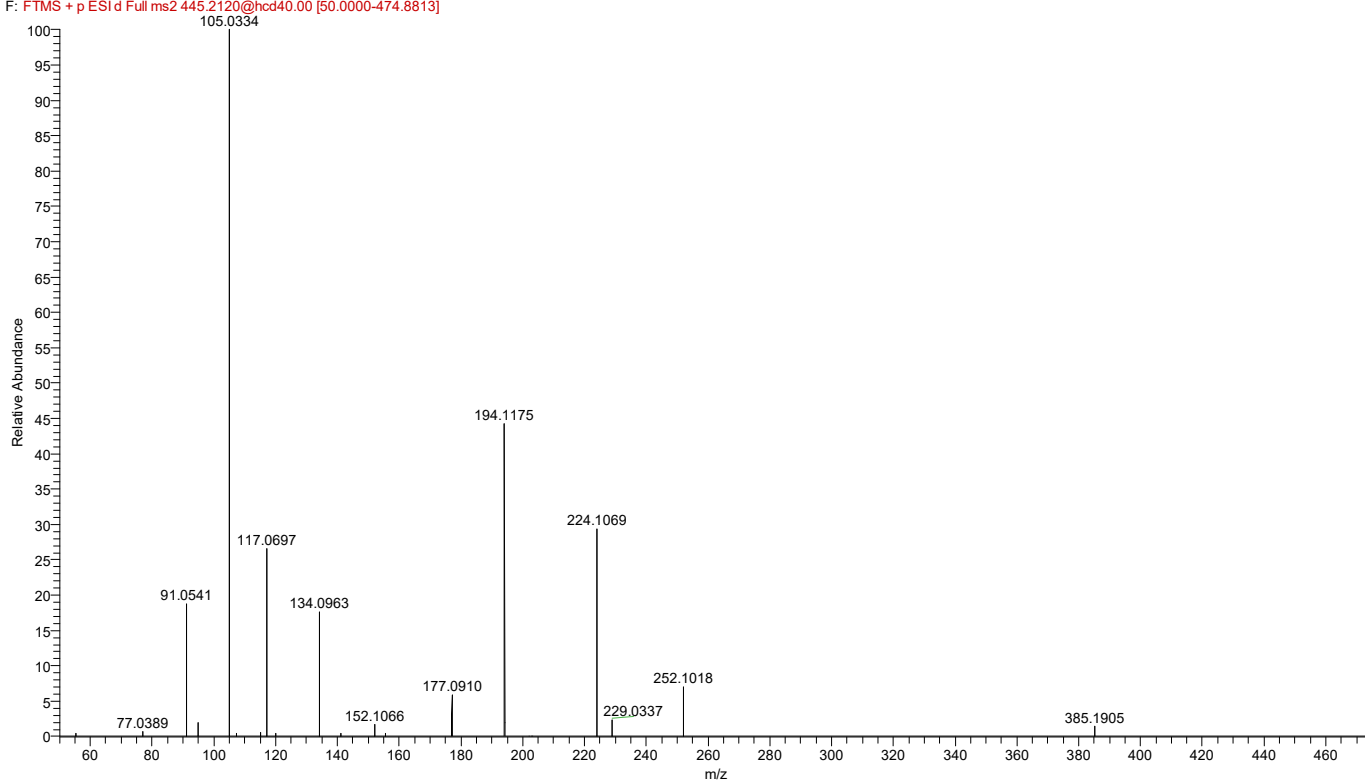
Figure S24. MS<sup>2</sup> fragmentation spectra (CID) of hematoxylin

ANX-100%JC-Pd #23704 RT: 20.66 AV: 1 NL: 1.72E6  
F: FTMS + p ESI d Full ms2 287.0552@hcd40.00 [50.0000-313.5613]



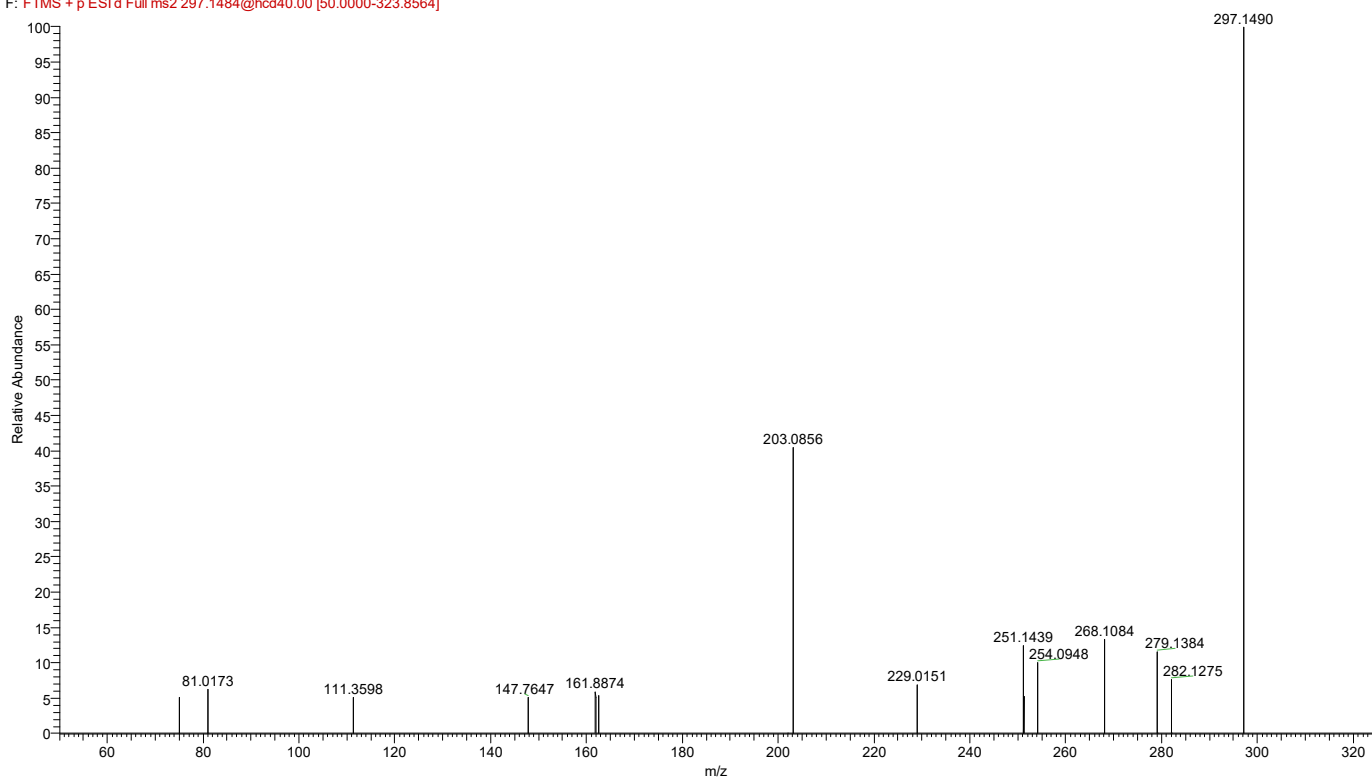
**Figure S25.** MS<sup>2</sup> fragmentation spectra (CID) of sakuranetin

ANX-100%JC-Pd #24688 RT: 21.51 AV: 1 NL: 8.11E6  
F: FTMS + p ESI d Full ms2 445.2120@hcd40.00 [50.0000-474.8813]



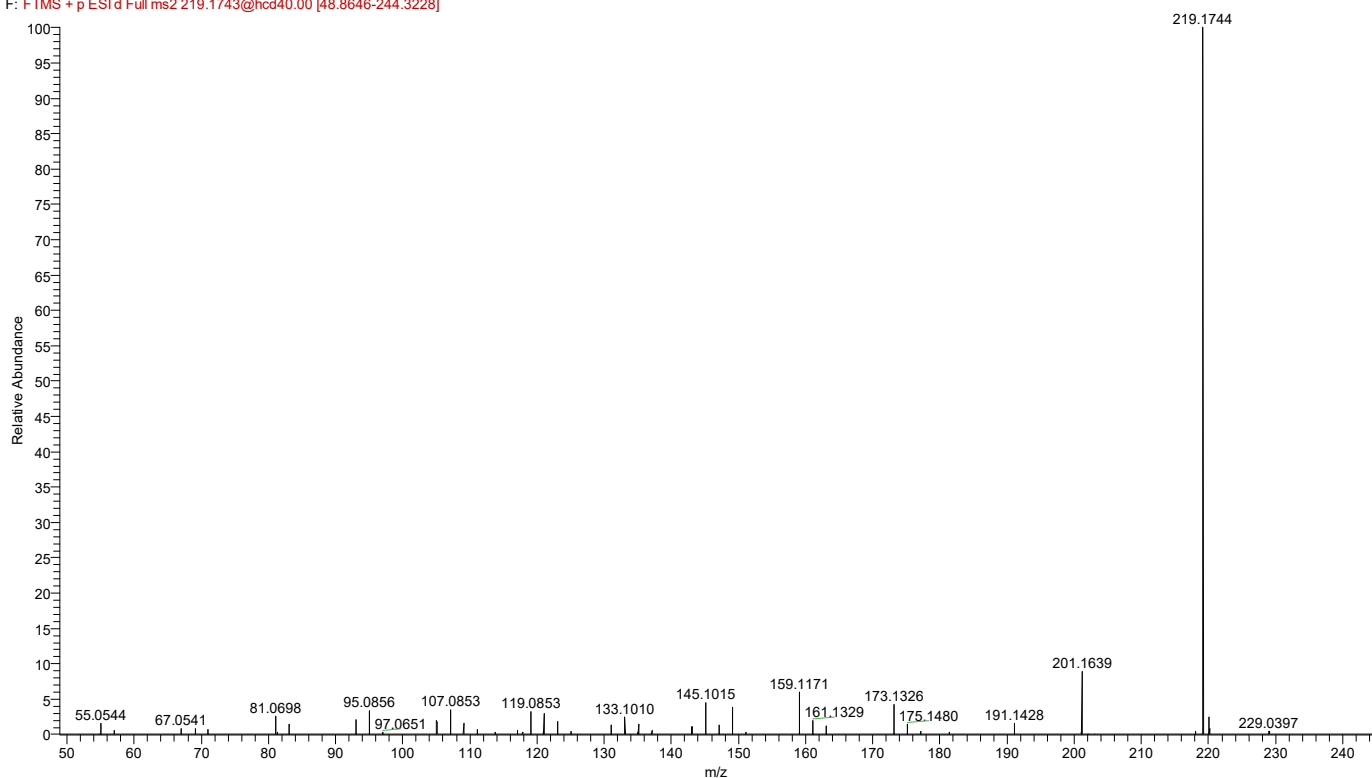
**Figure S26.** MS<sup>2</sup> fragmentation spectra (CID) of aurantiamide acetate

ANX-100%JC-Pd #26440 RT: 23.04 AV: 1 NL: 1.83E5  
F: FTMS + p ESI d Full ms2 297.1484@hcd40.00 [50.0000-323.8564]



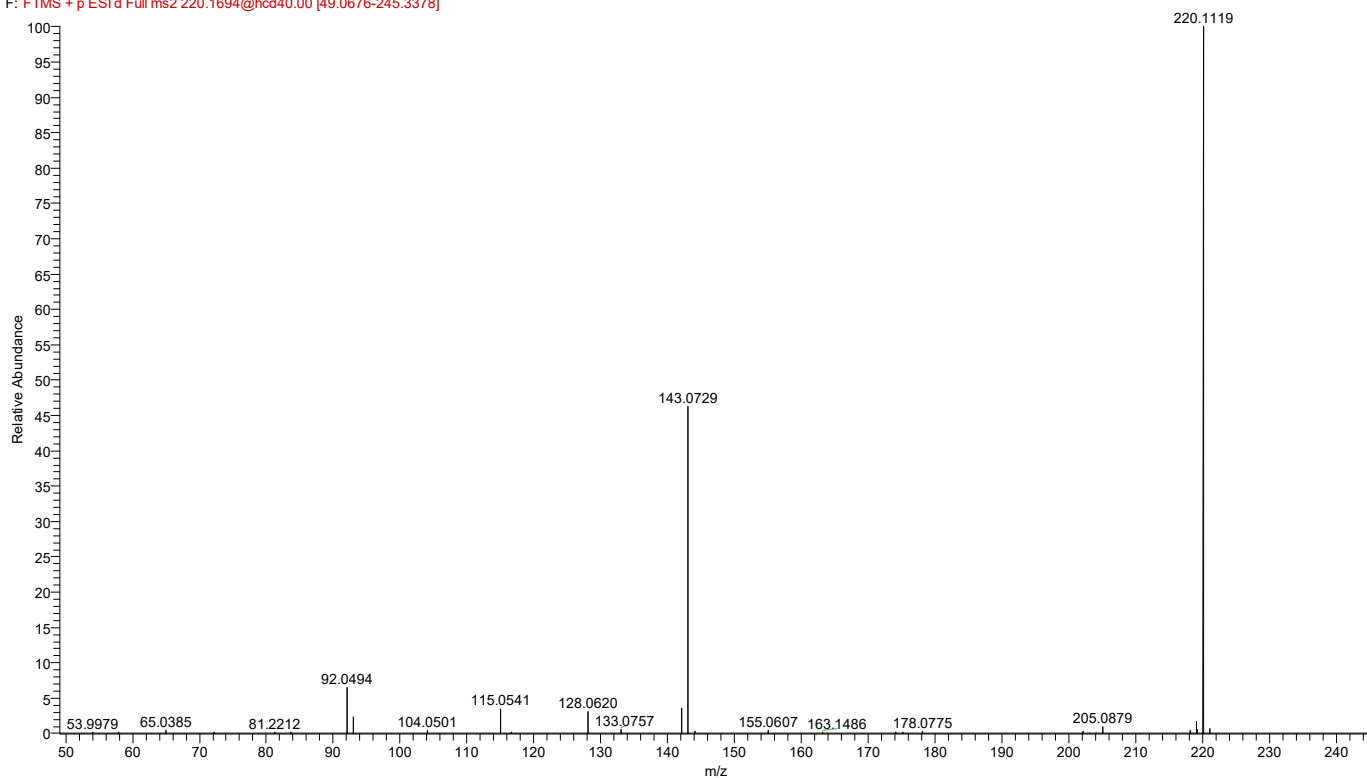
**Figure S27.** MS<sup>2</sup> fragmentation spectra (CID) of cryptotanshinone

ANX-100%JC-Pd #26678 RT: 23.24 AV: 1 NL: 1.05E6  
F: FTMS + p ESI d Full ms2 219.1743@hcd40.00 [48.8646-244.3228]



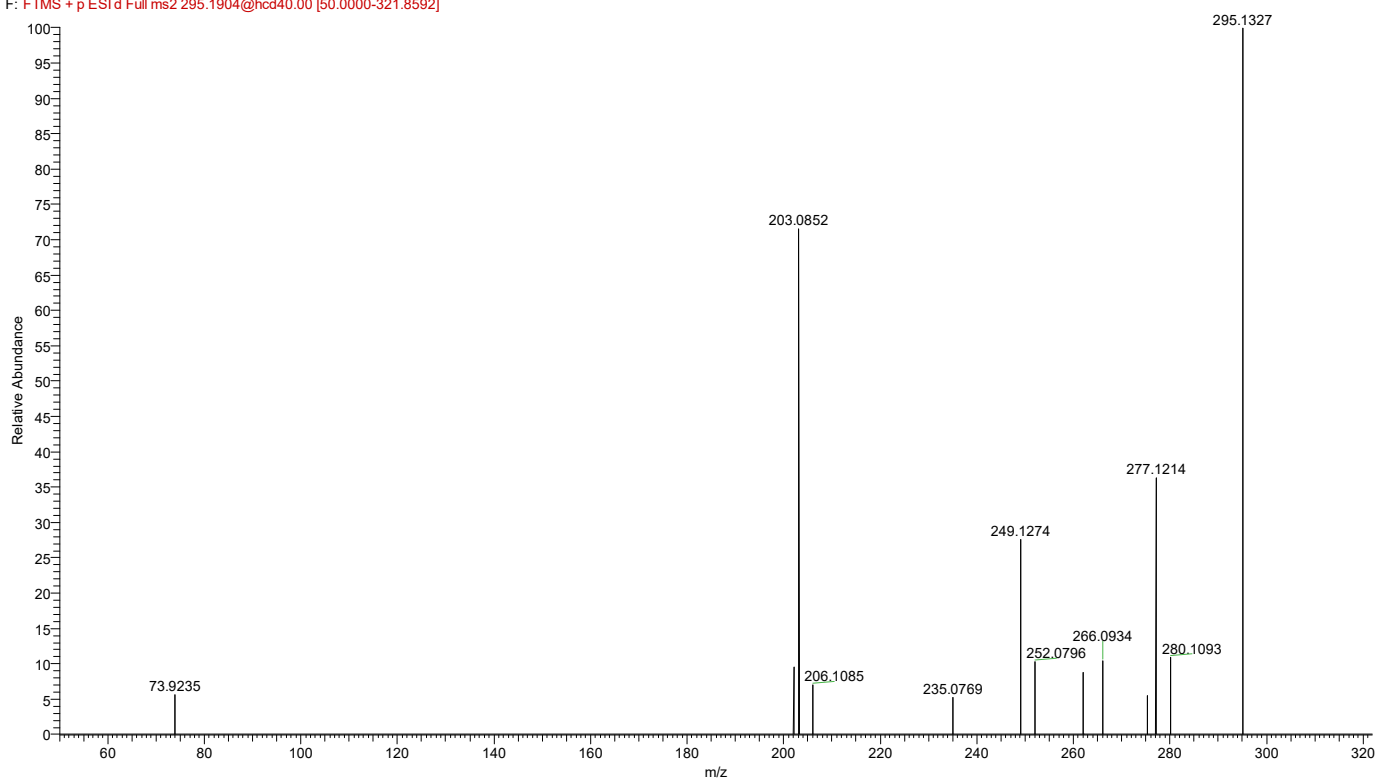
**Figure S28.** MS<sup>2</sup> fragmentation spectra (CID) of nootkatone

ANX-100%JC-Pd #26723 RT: 23.28 AV: 1 NL: 1.85E6  
F: FTMS + p ESI d Full ms2 220.1694@hcd40.00 [49.0676-245.3378]



**Figure S29.** MS<sup>2</sup> fragmentation spectra (CID) of N-Phenyl-1-naphthylamine

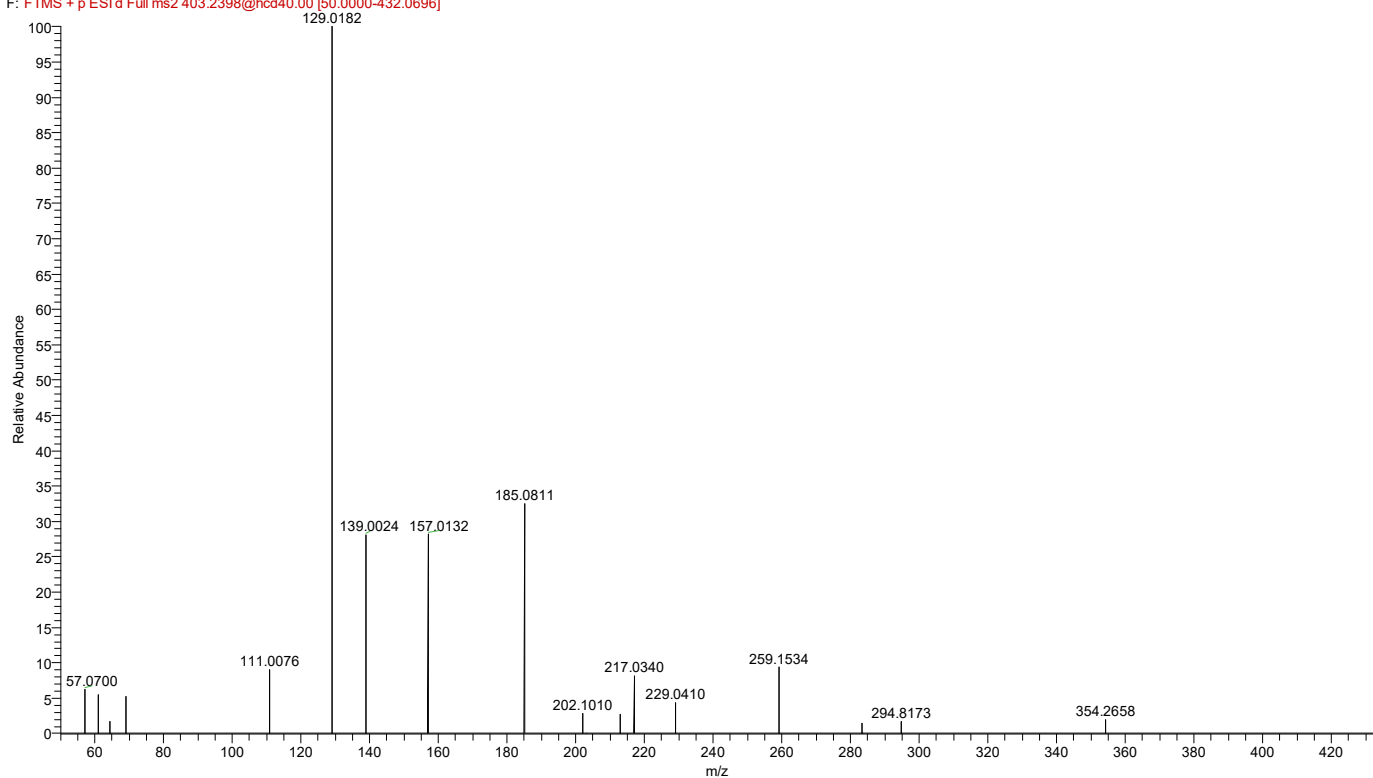
ANX-100%JC-Pd #27625 RT: 24.07 AV: 1 NL: 2.00E5  
F: FTMS + p ESI d Full ms2 295.1904@hcd40.00 [50.0000-321.8592]



**Figure S30.** MS<sup>2</sup> fragmentation spectra (CID) of tanshinone IIA

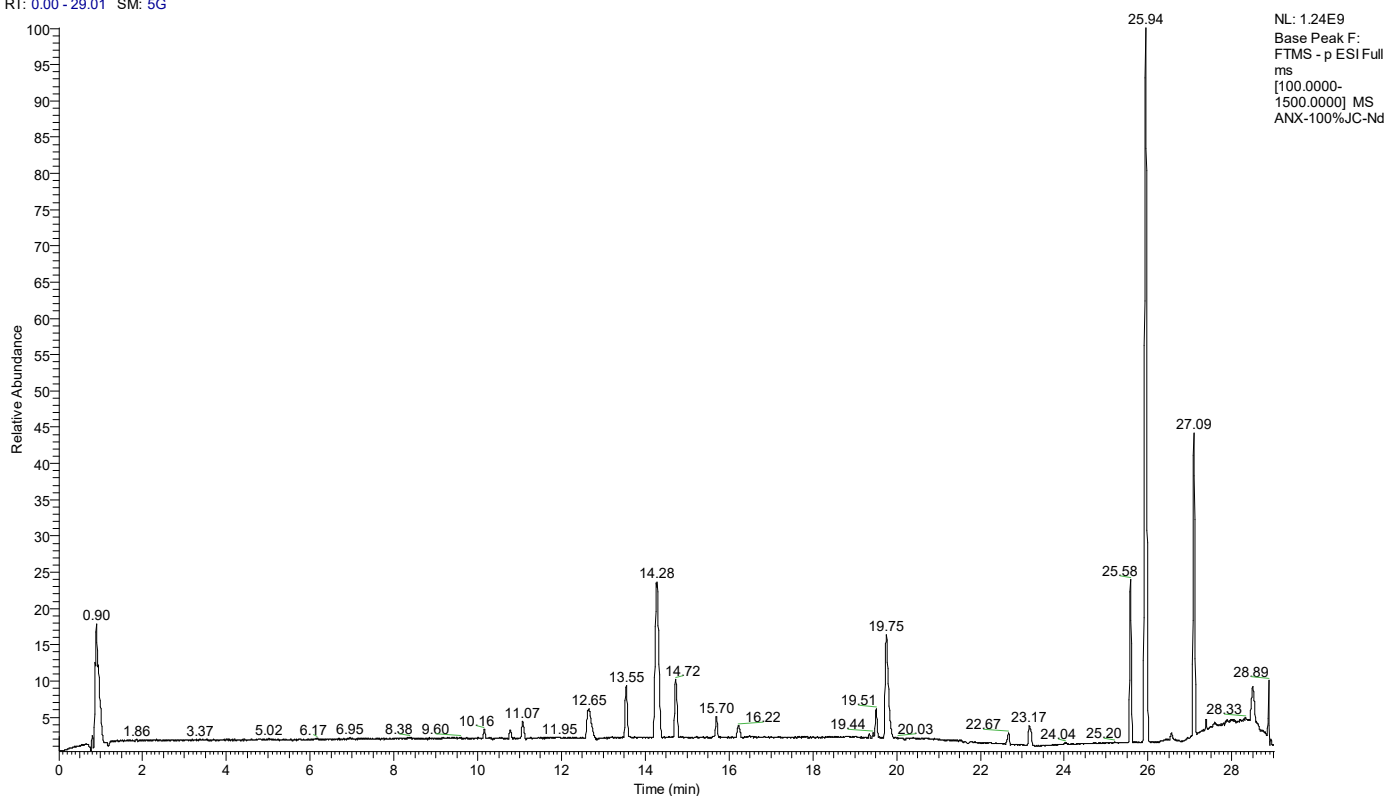


ANX-100%JC-Pd #28354 RT: 24.70 AV: 1 NL: 6.52E5  
 F: FTMS + p ESI d Full ms2 403.2398@hcd40.00 [50.0000-432.0696]



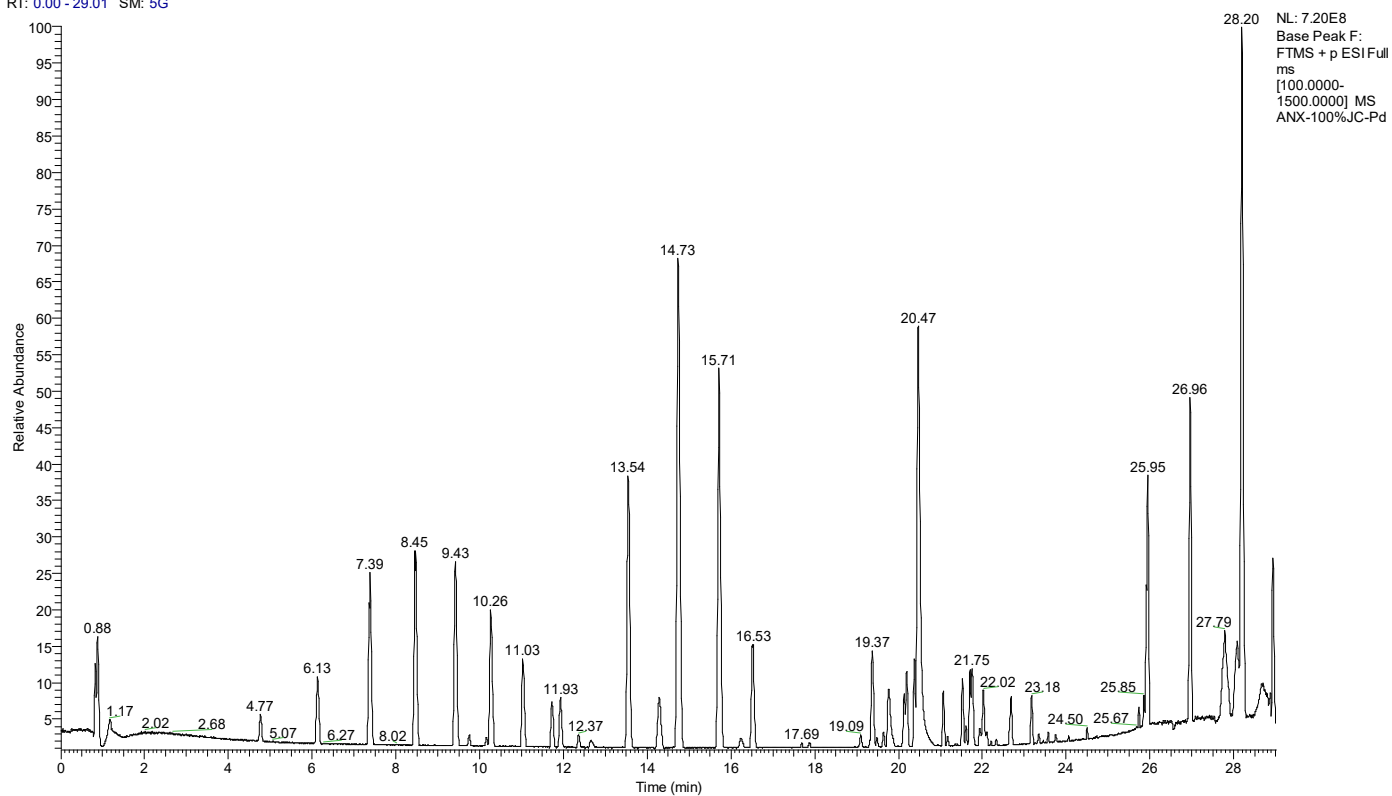
**Figure S31.** MS<sup>2</sup> fragmentation spectra (CID) of citroflex A-4

RT: 0.00 - 29.01 SM: 5G



**Figure S32.** TICs of *Blumea balsamifera* (L.) DC. in negative ion mode

RT: 0.00 - 29.01 SM: 5G



**Figure S33.** TICs of *Blumea balsamifera* ( L. ) DC. in positive ion mode