Angelica Stem: A Potential Low-cost Source of Bioactive Phthalides and Phytosterols

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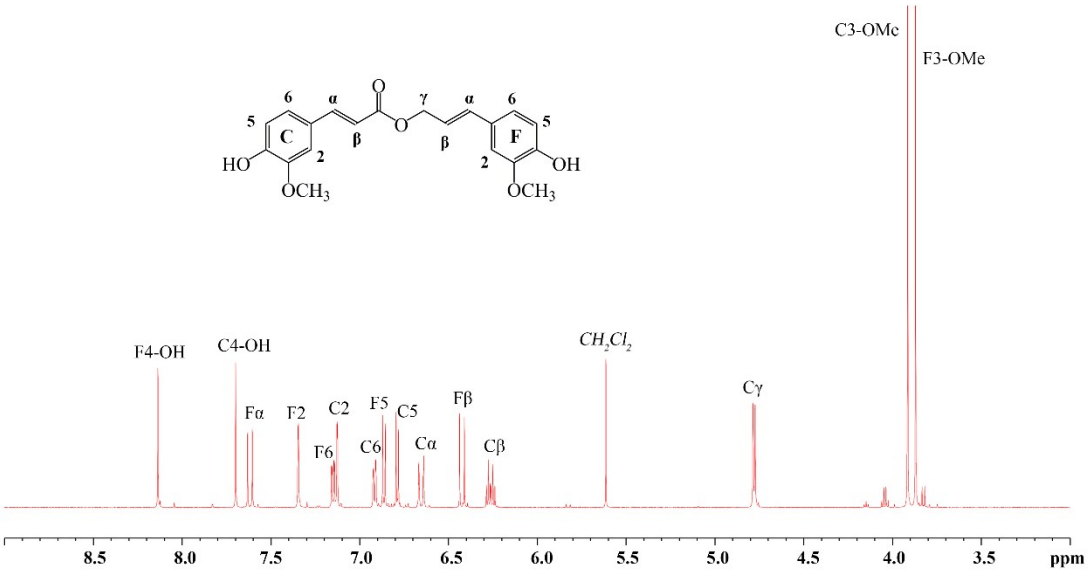


Figure S1. ^{1}H NMR of coniferyl ferulate.

Table S1. GC-MS program for analyzing derivatized extracts of angelica sinensis.

Gas Chromatograph	GC-2010 Plus
Inlet	200 °C Split liner with glass wool (Shimadzu 220-90784-00) Split injection (20:1)
Column	SH-Rxi-5Sil MS 30 m x 0.25 mm x 0.25 µm (Restek 13623) Helium carrier gas Constant linear velocity 47.2 cm/sec
Oven Program	50 °C, ramp 8 °C/minute to 150 °C, 5 °C/minute to 230 °C, 10°C/minute to 280 °C, hold 20 minutes MS interface 280 °C Analysis time 55 minutes
Mass Spectrometer	GCMS-TQ8040
Ion Source	200 °C Electron ionization (EI) mode, 70 eV
Operation Mode	Q3 scan
Detector	Electron multiplier 1.6 kV

Table S2. LC-MS/MS program for analysis of coniferyl ferulate and ferulic acid.

LC Chromatograph	Nexera UHPLC system						
Injector	SIL-20AXR Inject 1μL						
Pump	Binary high-pressure gradient system Mobile phase: Acetonitrile-aqueous (with 0.1% acetic acid) Total flow rate 0.4 mL/min						
Time program	0-2 min 5% acetonitrile; 2-6 min linear gradient to 40% acetonitrile; 6-10 min linear gradient to 80% acetonitrile; 10-15 min isocratic elution 80% acetonitrile; 15.1 -18 min 5% acetonitrile.						
Column	Shim-pack GISS C18 Column SH-Rxi-5Sil MS 50 mm x 2.1 mm x 1.9 μm						
Oven Program	CTO-20AC, 30 °C						
Mass Spectrometer	LCMS-TQ8050						
Interface	Electronic Spray Ion (ESI) mode Gasl 3 L/min; drying gas 10 L/min Interface 200 °C; DL250 °C; Heating block 300 °C						
Operation Mode	Multiple Reaction Monitoring (MRM), negative ion mode Argon gas, 17 kPa Ion range 80-500 (m/z) Event time 0.309 s; total measure time 15 min						
MRM Transition Details							
Compound Name	Retention time (min)	Transition 1	CE 1	Transition 2	CE 2	Transition 3	CE 3
Ferulic acid	5.12	193>178.2	14	193>134.1	14	193>133.1	25
Coniferyl ferulate	8.04	193>178.2	14	193>134.1	14	193>133.1	25

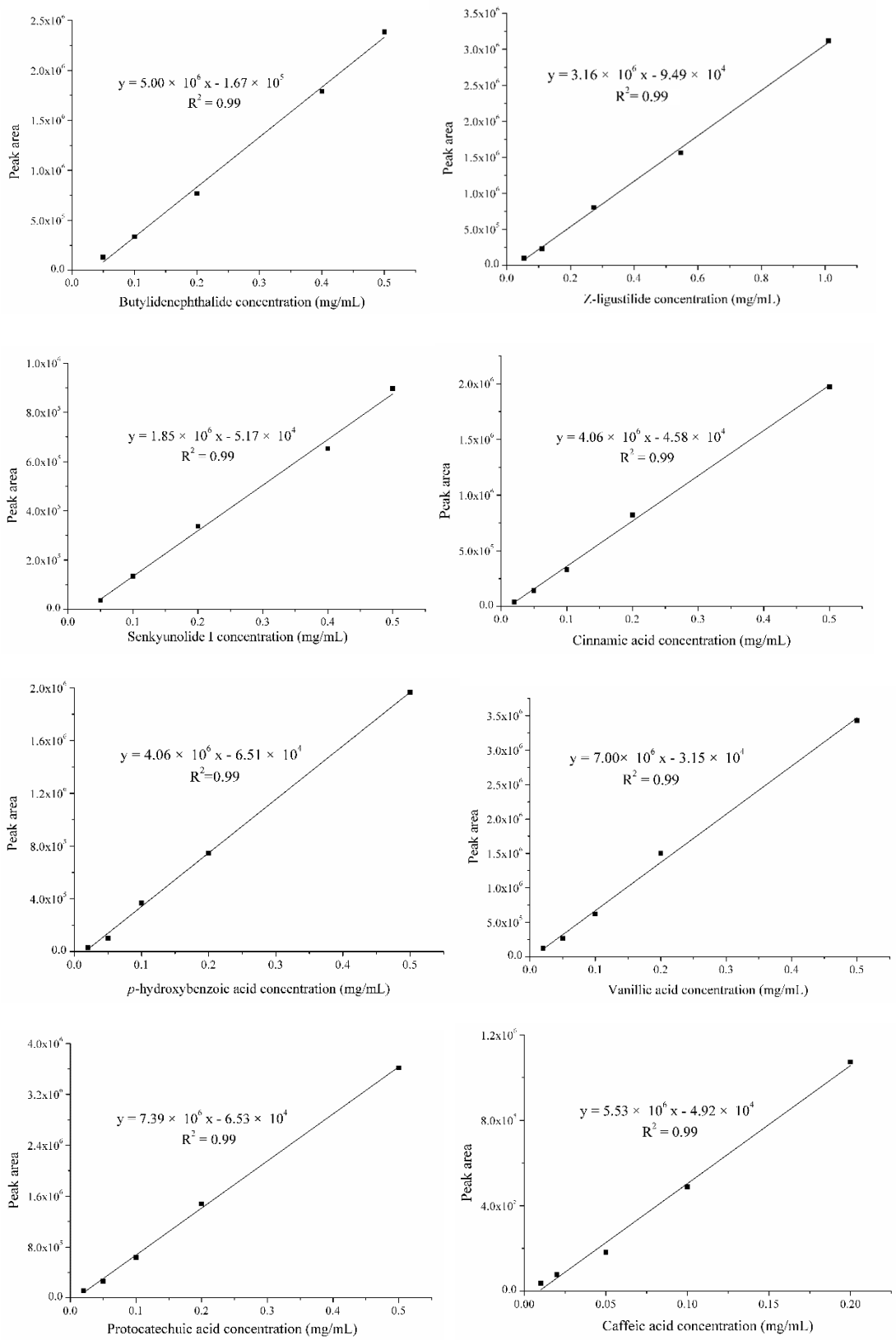
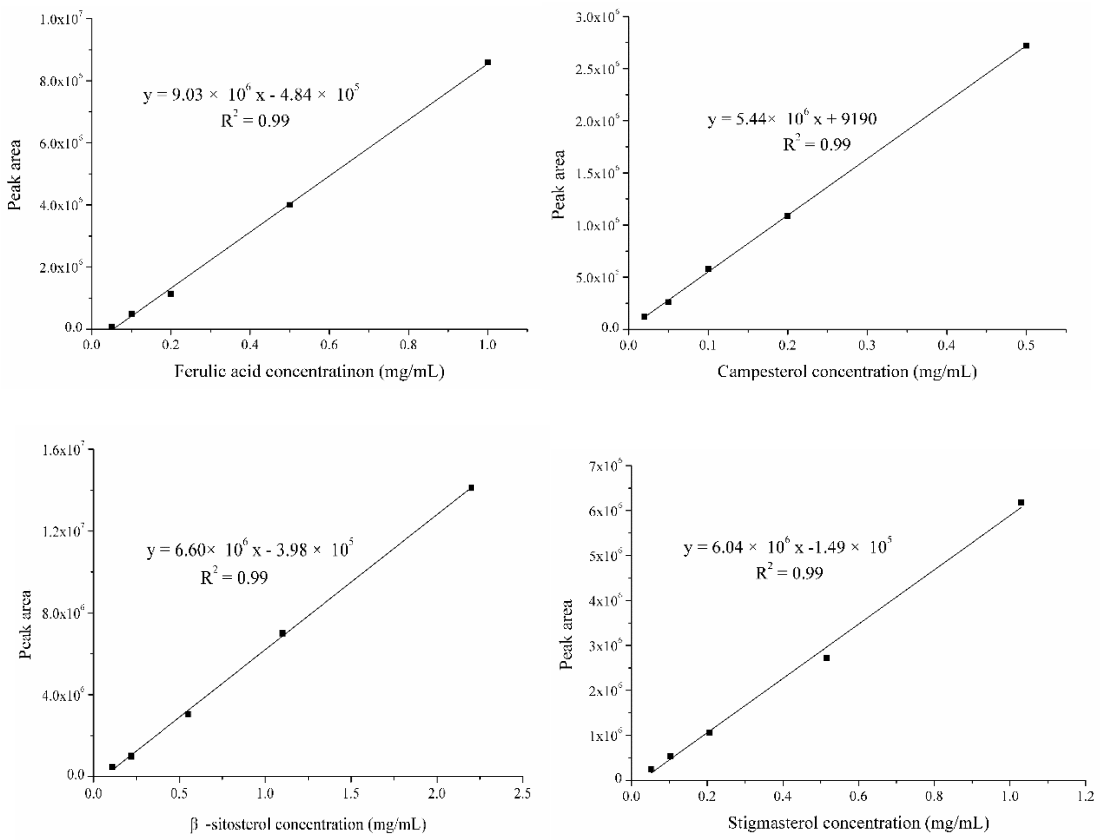


Figure S2. Linear regression equations for calculation of bioactive compounds identified in GC chromatograms (continued).



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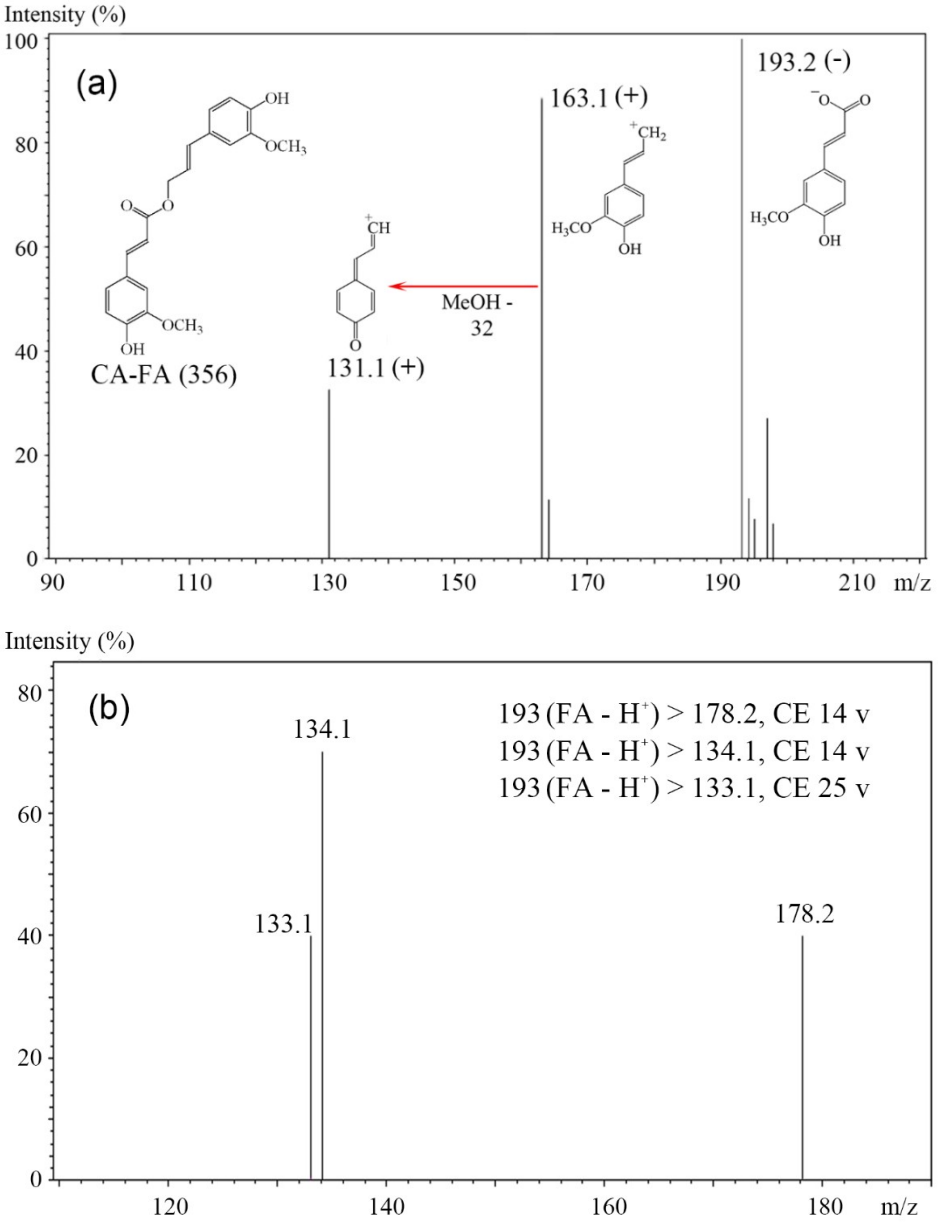

Figure S3. MS spectrum of coniferyl ferulate (CA-FA) (a) and the optimized MS fragmentations and corresponding optimal collision energys (CE) for $[FA-H]^-$ (m/z 193) ion in MRM mode (b).

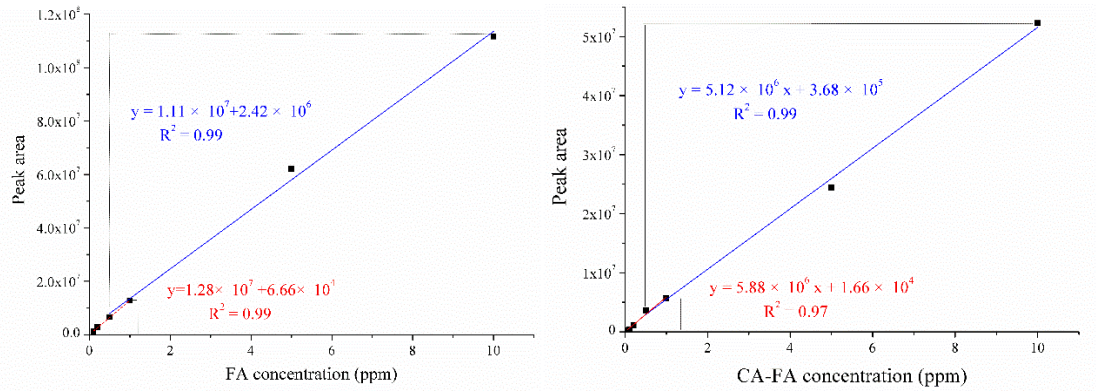

Figure S4. Linear regression equations of ferulic acid (FA) and coniferyl ferulate (CA-FA) in LC chromatograms.

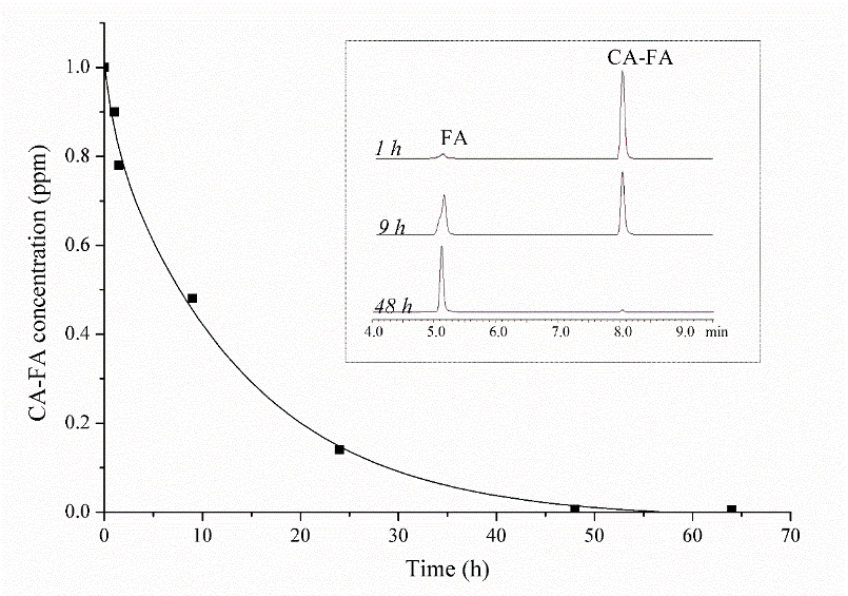

Figure 5. Degradation of coniferyl ferulate in methanol solution (temperature 25 °C). FA is ferulic acid, CA-FA is coniferyl ferulate.