

Figure S1. Temperature conditions (A), relative humidity (B), and daylight hours (C) in Chungnam National University, Daejeon, Korea (36°22'08.0" N 127°21'14.2" E)

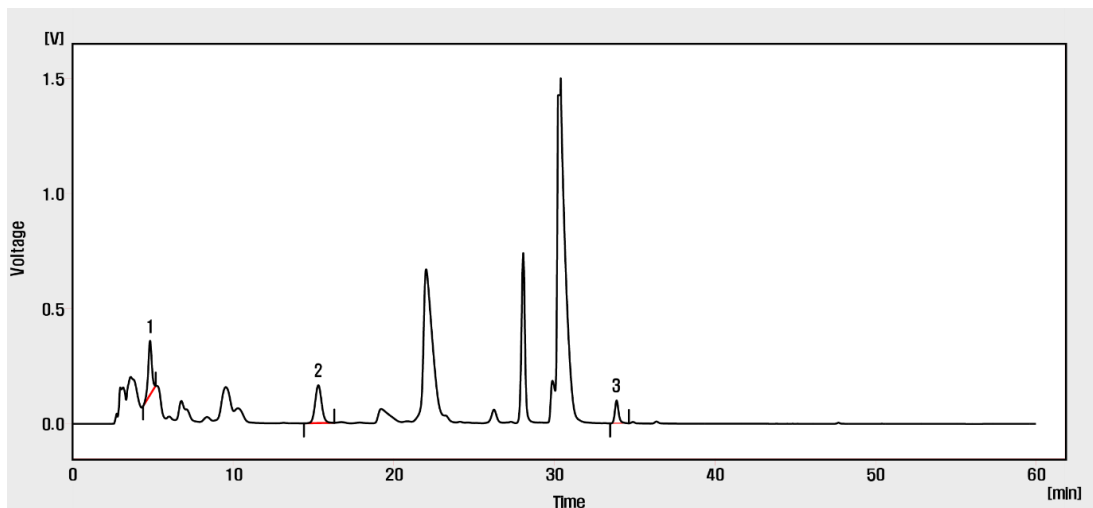


Figure S2. Representative chromatogram of rosmarinic acid, tilianin, and acacetin obtained from freeze-dried *Agastache rugosa*. Peak: 1. Rosmarinic acid; 2. Tilianin; 3. Acacetin.

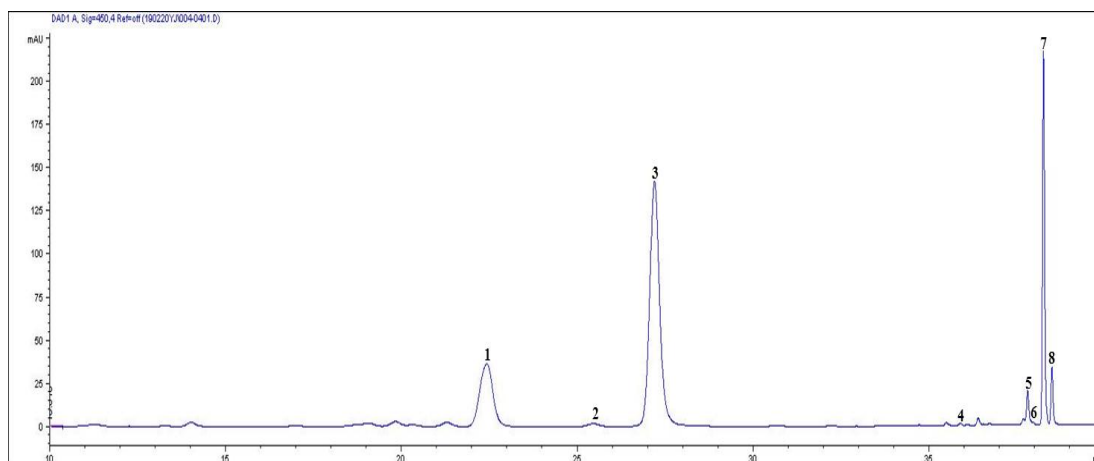


Figure S3. Representative chromatogram of carotenoids obtained from freeze-dried *Agastache rugosa*. Peak: 1. Lutein; 2. Zeaxanthin; 3. *trans*- β -apo-8'-carotenal (internal standard); 4. β -Cryptoxanthin; 5. 13Z- β -Carotene; 6. α -Carotene; 7. β -Carotene; 8. 9Z- β -Carotene.

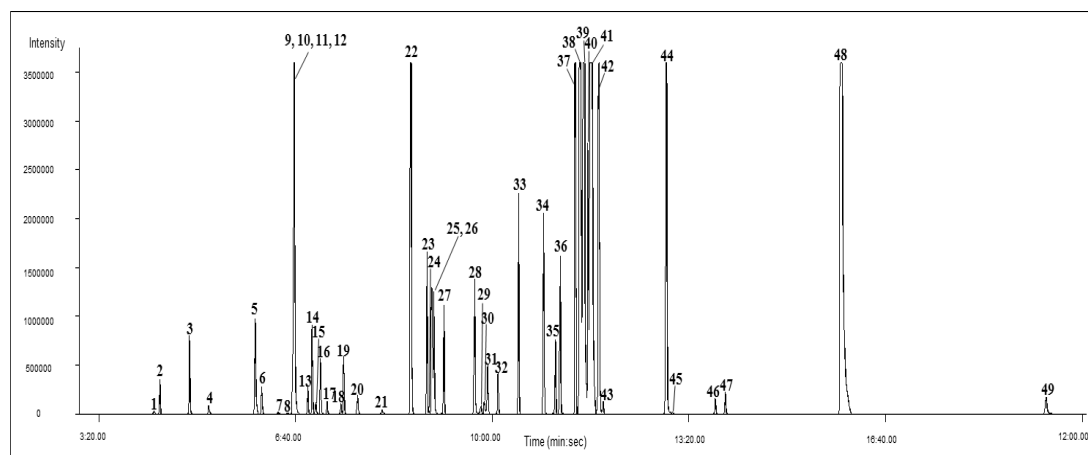


Figure S4. Representative chromatogram of metabolites obtained from freeze-dried *Agastache rugosa*. Peak: 1, Pyruvic acid; 2, Lactic Acid; 3, Alanine; 4, Oxalic acid; 5, Glycolic acid; 6, Valine; 7, Urea; 8, Ethanolamine; 9, Phosphoric acid; 10, Glycerol; 11, Leucine; 12, Isoleucine; 13, Proline; 14, Glycine; 15, Succinic Acid; 16, Glyceric Acid; 17, Fumaric Acid; 18, Serine; 19, Threonine; 20, β -Alanine; 21, Malic acid; 22, Aspartic Acid; 23, Methionine; 24, Pyroglutamic Acid; 25, 4-Aminobutyric Acid; 26, Threonic acid; 27, Glutamic Acid; 28, Phenylalanine; 29, Xylose-1; 30, Xylose-2; 31, Asparagine; 32, Ribitol (internal standard) 33, Glutamine; 34, Shikimic acid; 35, Citric acid; 36, Quinic acid; 37, Fructose-1; 38, Fructose-2; 39, Galactose; 40, Glucose-1; 41, Glucose-2; 42, Mannitol; 43, Inositol; 44, Ferulic acid; 45, Tryptophan; 46, Sinapinic acid; 47, Sucrose; and 48, Raffinose.

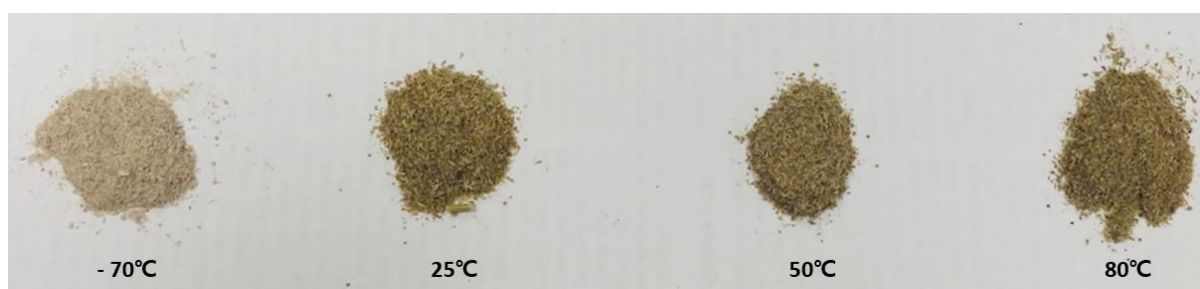


Figure S5. *Agastache rugosa* flower samples were dried using four different methods (oven drying at 25 ± 1 °C, 50 ± 1 °C, 80 ± 1 °C, and freeze drying).

Table S1. HPLC and GC-TOFMS analysis methods.

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| HPLC analysis method for polyphenols | HPLC system | An NS-4000 HPLC system (Futecs Co., Daejeon, South Korea) with a UV-Vis detector, a NS-6000 autosampler (Futecs Co., Daejeon, South Korea) |
| | Column | OptimaPak C18 column (250 × 4.6 mm, 5 μm, RStech Co., Daejeon, South Korea) |
| | UV wavelength | 280 nm |
| | Flow rate | 1.0 mL/min |
| | Injection volume | 20 μL |
| | Column temperature | 30°C. |
| HPLC analysis method for carotenoids | HPLC system | HPLC system (Agilent 1000) equipped with PDA-detector (450 nm) |
| | Column | C30 YMC column (250 × 4.6 mm, 3 μm; Waters Corporation, Milford, MA, USA) |
| | UV wavelength | 450 nm |
| | Flow rate | 1.0 mL/min |
| | Injection volume | 20 μL |
| | Column temperature | 40°C. |
| GC-TOFMS analysis method for primary metabolites | Agilent 7890A gas chromatograph (Agilent, Atlanta, GA, USA) combined with a Pegasus HT TOF mass spectrometer (LECO, St. Joseph, MI, USA). The gas chromatograph was equipped with a CP-Sil 8 CB low bleed/MS fused-silica capillary column (5% phenyl/95% dimethylpolysiloxane, 60 m × 0.25 mm ID, 0.25-μm film thickness; Varian Inc., Palo Alto, CA, USA). The operating conditions were set as follow: injection port temperature, 230 °C; helium gas flow rate, 1.0 mL min ⁻¹ ; split ratio, 1:25. The temperature program was set as follows: initial temperature of 80 °C, 2 min; an increase to 320 °C at 15 °C/min; 10 min heating at 320 °C; transfer line temperature, 250 °C; the ion source temperatures, 200 °C; the scanned mass range, m/z 85–600; and the detector voltage, 1700 V. | |