

Chemical Information:

Name: Chlorogenic acid
CAS No.: 327-97-9
Tox21_ID No.: Tox21_202495
NTP_CID No.: 620

Supplier: Acros Organics
Lot No.: A0260877
MW: 354.30 g/mol

Dates of Analysis:

LC/UV: 25 January 2017
LC/MS: 05 January 2017

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Chlorogenic acid	2.51	100.00

^a Peaks comprising $\geq 0.5\%$ of total area.

Instrument Parameters:

Instrument / Ionization	Shimadzu UPLC; Micromass Quattro II / ESI-
Solvent	Methanol
Column	Grace Alltima C18, 5 μ m, 250 mm x 4.6 mm ID
Injection Volume / Detection	10 μ L / 225 nm
Mobile Phase	Water (A) / Acetonitrile (B)
Program / Flow Rate	50/50 A/B for 40 minutes; 0/100 in 10 minutes, hold 10 minutes; 50/50 for 15 minutes / 1.0 mL/minute
Cone / Corona	50 V / 3.0 kV
Source Temperature	125°C
Probe Temperature	350°C
Scan Range	20 – 1300 amu
Acquisition Software	LC/UV – LabSolutions, v 5.71.SP1; LC/MS – MassLynx 4.0

