

Chemical Information:

Name: Yangonin

Date of Analysis: 05 October 2010

CAS No.: 500-62-9

Supplier: ChromaDex

Tox21_ID No.: Tox21_202547

Lot No.: 25010-02082007

NTP_CID No.: 1402

MW: 258.27 g/mol

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
unknown	29.6	6.0
Yangonin	30.1	94.0

^a Peaks comprising ≥ 0.5% of total area.

LC/MS Instrument Parameters:

Instrument / Ionization	Micromass Quattro II with Shimadzu HPLC / ESI+
Solvent	Methanol
Column	Grace HP C18-AQ, 5 µm, 250 mm x 2.1 mm ID
Injection Volume	20 µL
Mobile Phase	95/5 (A) and 5/95 (B) Water/acetonitrile 2 mM ammonium formate, pH 3; acetonitrile (C)
Program / Flow Rate	100/0/0 A/B/C for 1 min; 0/100/0 at 35 min, hold 2 min; 0/0/100 at 37.1 min, hold 3 min; 100/0/0 at 40 min, hold 5 min / 0.2 mL/min
Cone / Capillary	25 V / 3.0 kV
Source Temperature	125°C
Desolve Temperature	325°C
Scan Range	125 – 1100 amu
Acquisition Software	MassLynx, v 4.0

