

Chemical Information:

Name: 5,7-Dihydroxy-4-methylcoumarin
CAS No.: 2107-76-8 Supplier: Sigma Aldrich
Tox21_ID No.: Tox21_200882 Lot No.: 15116AO
NTP_CID No.: 399 MW: 192.17 g/mol

Date of Analysis: 24 August 2009

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
5,7-Dihydroxy-4-methylcoumarin	19.49	100

^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	15 µL
Mobile Phase	Water (A) / methanol (B)
Program / Flow Rate	95/5 A/B for 1 minute; 10/90 in 20 minutes, hold 1 minute / 0.2 mL/minute
Cone / Corona	40 V / 3.5 kV
Source Temperature	140°C
Probe Temperature	325°C
Scan Range	120 – 1000 amu
Acquisition Software	MassLynx, v 4.0

