

Chemical Information:

Name: Phloretin

CAS No.: 60-82-2

Tox21_ID No.: Tox21_202854

NTP_CID No.: 6249

Supplier: Sigma-Aldrich

Lot No.: 080M7011V

MW: 274.27 g/mol

Dates of Analysis:

LC/UV: 04 January 2017

LC/MS: 23 December 2016

Purity and Identity Results:

| Peak Identity | Retention Time (min) | Purity (% Total Area) ^a |
|---------------|----------------------|------------------------------------|
| Phloretin | 4.83 | 99.71 |

^a Peaks comprising ≥ 0.5% of total area.

Instrument Parameters:

| | |
|------------------------------|--|
| Instrument / Ionization | Shimadzu UPLC; Micromass Quattro II / ESI+ |
| Solvent | Acetone |
| Column | Grace Alltima C18, 5 µm, 250 mm x 4.6 mm ID |
| Injection Volume / Detection | 10 µL / 254 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 – 1000 amu |
| Acquisition Software | LC/UV – LabSolutions, v 5.71.SP1; LC/MS – MassLynx 4.0 |

