

### Chemical Information:

Name: Rutin trihydrate  
CAS Nos.: 153-18-4  
250249-75-3  
Tox21\_ID No.: Tox21\_202602  
NTP\_CID No.: 4865

Supplier: Sigma-Aldrich  
Lot No.: 1380505  
MW: 664.56 g/mol

Dates of Analysis:  
LC/UV: 18 November 2017  
LC/MS: 01 February 2017

### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Unknown	2.07	1.10
Unknown	3.74	0.62
Rutin	8.28	98.28

<sup>a</sup> Peaks comprising ≥ 0.5% of total area.

### LC/MS and LC/UV Instrument Parameters:

Instrument / Ionization	Shimadzu UPLC; Micromass Quattro II / ESI+
Solvent	Methanol
Column	Grace Alltima C18, 5 µm, 250mm x 4.6mm ID
Injection Volume / Detection	10 µL / 215 nm
Mobile Phase	Water (A) / Methanol (B)
Program / Flow Rate	50/50 A/B for 20 minutes; 0/100 in 10 minutes, hold 10 minutes; 50/50 for 25 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

