

# Chemical Information:

Name: Celecoxib  
CAS No.: 169590-42-5  
Tox21\_ID No.: Tox21\_201964  
NTP\_CID No.: 606

Date of Analysis: 17 July 2009  
Supplier: LKT Laboratories, Inc.  
Lot No.: 010404  
MW: 381.37 g/mol

## Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Celecoxib	21.62	100

<sup>a</sup> 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	Water (A) / acetonitrile (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 / 3.0 kV
Source Temperature	140°C
Probe Temperature	325°C
Scan Range	85 – 1400 amu
Acquisition Software	MassLynx, v 4.0

