

Chemical Information:

Name: Silybin
CAS No.: 22888-70-6
Tox21_ID No.: Tox21_200755
NTP_CID No.: 1273

Supplier: Sigma Aldrich
Lot No.: 044K0845
MW: 482.44 g/mol

Date of Analysis: 20 November 2009

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Silibinin	16.5	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	20 µL
Mobile Phase	95/5 (A) and 5/95 (B) Water/acetonitrile with 2 mM ammonium formate, pH 3
Program / Flow Rate	100/0 A/B for 1 minute; 5/95 in 20 minutes, hold 1 minute / 0.2 mL/minute
Cone / Capillary	25 V / 3.0 kV
Source Temperature	125°C
Desolve Temperature	300°C
Scan Range	125 – 1000 amu
Acquisition Software	MassLynx, v 4.0

