

Chemical Information:

Name: 3,4,5-Trichloronitrobenzene
CAS No.: 20098-48-0 Supplier: Sigma Aldrich
Tox21_ID No.: Tox21_200704 Lot No.: 19529CO
NTP_CID No.: 299 MW: 226.44 g/mol

Date of Analysis: 08 May 2009

Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
3,4,5-Trichloronitrobenzene	21.52	100

^a Peaks comprising ≥ 0.5% of total area.

LC/MS Instrument Parameters:

Instrument / Ionization	Micromass Quattro II with Shimadzu HPLC / APCI-
Solvent	Methanol
Column	Grace HP C18-AQ, 5 µm, 250 mm x 4.6 mm ID
Injection Volume	50 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 / 1 mL/minute
Cone / Corona	25 V / 3.0 kV
Source Temperature	125°C
Probe Temperature	300°C
Scan Range	70 – 850 amu
Acquisition Software	MassLynx, v 4.0

