

### Chemical Information:

Name: Phenyl isothiocyanate  
CAS No.: 103-72-0  
Tox21\_ID No.: Tox21\_201128  
NTP\_CID No.: 4644

Supplier: Alfa Aesar  
Lot No.: E24S046  
MW: 135.19 g/mol

Date of Analysis: 04 September 2015

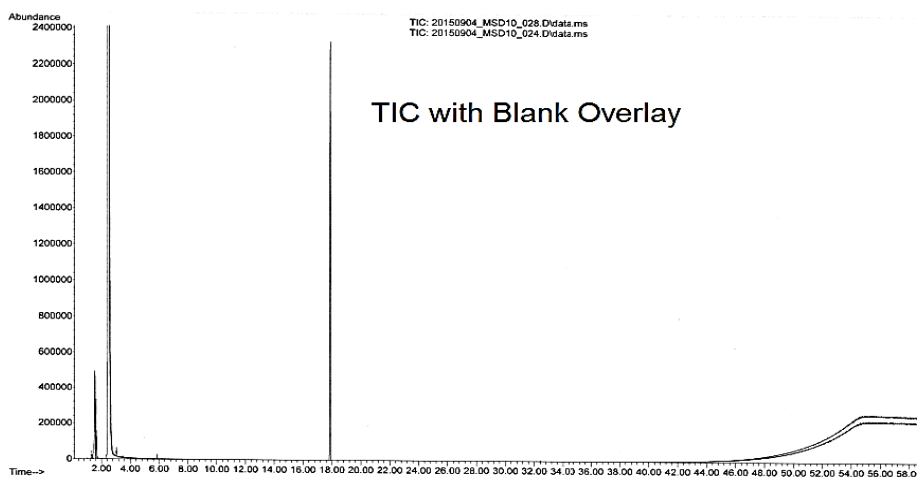
### Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) <sup>a</sup>
Phenyl isothiocyanate	17.87	99.92

<sup>a</sup> Peaks comprising  $\geq 0.5\%$  of total area.

### GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Chloroform
Column	Rtx-5 MS, 30 m x 0.25 mm ID, 1- $\mu$ m film thickness
Carrier Gas	Helium at 2.0 mL/min
Oven Program	50°C, hold 0 min; ramp @ 5°C/min to 320°C, hold 5 min
Source Temperature	230°C
Auxiliary Temperature	250°C
Scan Range	40 – 575 amu
Injector Temperature	250°C
Injection Volume / Mode	1 $\mu$ L / Split (10:1)
Data Analysis Software	MSD ChemStation, ver F.01.01.2317, NIST Library ver 2.2f, build Dec 2014



Unknown: Scan 2917 (17.868 min): 20150904\_MSD10\_028.D\data.ms  
Compound in Library Factor = 454

Hit 1: Benzene, isothiocyanato-  
C7H5NS; MF: 936; RMF: 936; Prob 54.4%; CAS: 103-72-0; Lib: mainlib; ID: 96440.

