

Chemical Information:

Name: 1,2-Benzenedicarboxylic acid, di-C6-8-branched alkyl esters, C7-rich
 Date of Analysis: 30 August 2015
 CAS No.: 71888-89-6 Supplier: Sigma-Aldrich
 Tox21_ID No.: Tox21_200941 Lot No.: 04516HJ
 NTP_CID No.: 3550 MW: 362.50 g/mol

Purity and Identity Results:

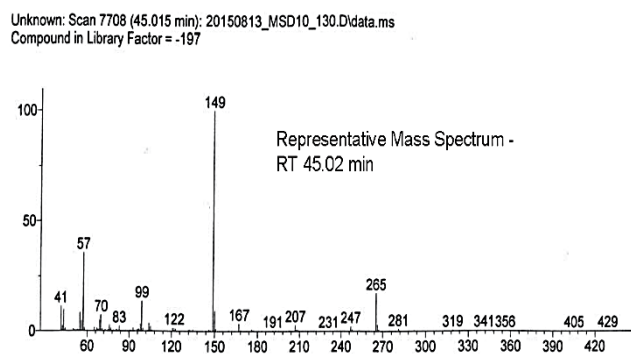
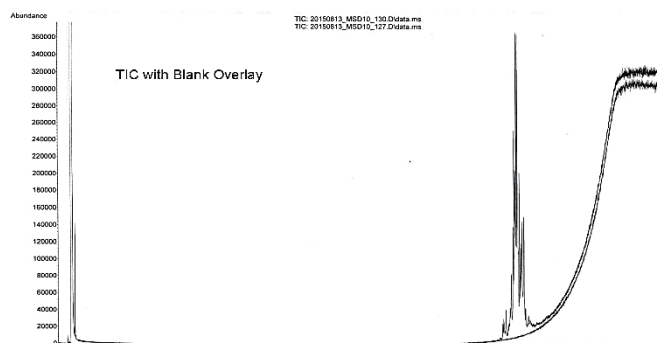
Peak Identity ^a	Retention Time (min)	Purity (% Total Area) ^b	Peak Identity ^a	Retention Time (min)	Purity (% Total Area) ^b
NIST ID 136946	44.60	6.36	NIST ID 137110	45.02	16.44
NIST ID 137110	44.70	11.10	NIST ID 137110	45.22	8.16
NIST ID 136946	44.80	9.50	NIST ID 137110	45.46	7.55
NIST ID 137110	44.91	14.09	NIST ID 137110	45.66	7.00

^a Per CoA, Diisooheptyl phthalate (mixture of C7 isomers), technical grade. Analysis yielded a number of unresolved components between 43.5 and 46.0 minutes. Based on mass spectra, components were identified as NIST ID 136946 (phthalic acid, 4,4-dimethylpent-2-yl heptyl ester) or NIST ID 137110 (phthalic acid, 5-methylhex-2-yl heptyl ester), indicating isomers of 1,2-benzenedicarboxylic acid with predominantly C7 branched alkyl esters. In addition to the eight components listed above, ten components ranging from 0.58 to 4.56% were observed. Total of all components = 98.78% purity.

^b Peaks comprising ≥ 0.5% of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Ethanol (~ 0.4 mg/mL)
Column	Rtx-5 MS, 30 m x 0.25 mm ID, 1-μm 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 – 550 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μL / Split (10:1)
Data Analysis Software	MassHunter GC/MS Acquisition B.07.02.7938 / Chemstation Enhanced Data Analysis F.01.01.2317 / NIST Library Version 2.2 Build 2014



Hit 1: Phthalic acid, 5-methylhex-2-yl heptyl ester
C22H34O4; MF: 873; RMF: 917; Prob 24.2%; Lib: mainlib; ID: 137110.

Hit 2: Phthalic acid, 4,4-dimethylpent-2-yl heptyl ester
C22H34O4; MF: 853; RMF: 896; Prob 11.0%; Lib: mainlib; ID: 136946.

