

Certificate of Analysis

Benzyl bromide

PurTech Standard for GC

Product Number	PSI132	CAS No.	100-39-0
Brand	PureSynth	Lot No.	FRDHP
Molecular Formula	C ₇ H ₇ Br	Date of Mfg.	May.2022
Molecular Weight	171.04 g/mol	Date of Exp.	Apr.2026

Test	Specification	Result
Description	Colorless to light yellow liquid	Light yellow liquid
Assay (GC-FID)	≥ 99.5 %	99.75 %
Water (By KF)	NMT 0.1 %	0.0923 %
Identification by ¹ H NMR	Conforms to structure	Conforms
Identification by GC-MS	Conforms to molecular mass	Conforms
Identification by IR	Conforms to structure	Conforms

***Traceable to internal reference standard**

Storage Condition: Store at room temperature and keep container tightly closed.

Remark: The batch complies with the prescribed quality of the above specification.

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Assay by GC-FID

METHOD: G.C- FID conditions:

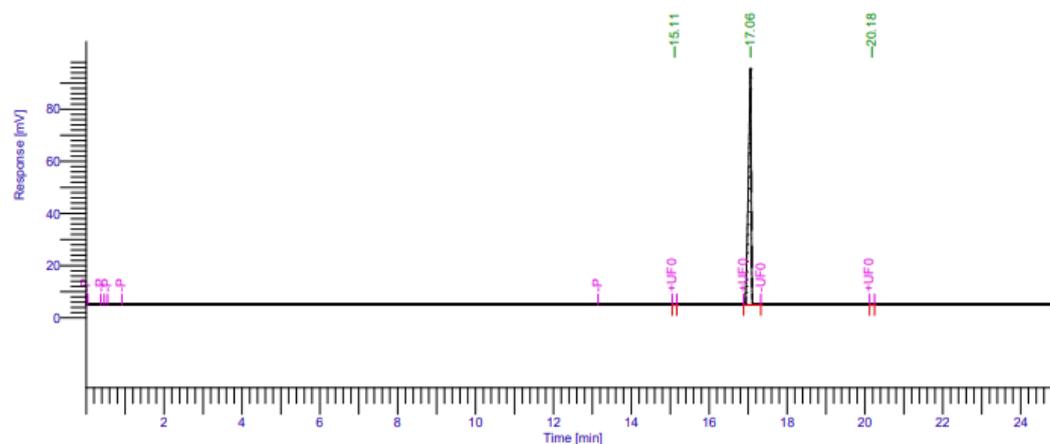
Column: Agilent Technologies DB-FFAP 30mx 0.530mm, 1.0micron

Instrument: PerkinElmer, GC 2014,

Detector: FID, **Carrier gas:** Nitrogen

Temp programming: Initial 50°C hold for 1min, 5°C Ramp/ min., 100 °C hold for 1 min., 25°C Ramp up to 250°C hold for 2 min., Run time 20 min.

Software Version : 6.3.4.0700	Date : 12/08/2022 3.14.20 PM
Operator : manager	Sample Name : AR22000379-BENZYL BROMIDE-FRD
Sample Number : 1	HP
AutoSampler : BUILT-IN	
Instrument Name : Clarus 680	Study : GC Purity
Instrument Serial # : None	Rack/Vial : 0/7
Delay Time : 0.00 min	Channel : A
Sampling Rate : 12.5000 pts/s	A/D mV Range : 1000
Sample Volume : 1.000000 ul	End Time : 25.00 min
Sample Amount : 1.0000	
Data Acquisition Time : 12/08/2022 1.46.29 PM	Area Reject : 0.000000
	Dilution Factor : 1.00
	Cycle : 1



GC Reports

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]
1		15.112	687.13	374.52	0.15
2		17.061	449318.87	90713.28	99.75
3		20.180	431.31	177.36	0.10
			450437.30	91265.15	100.00

Missing Component Report
Component Expected Retention (Calibration File)

All components were found

Purity by GC-FID: 99.75 %

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IDENTIFICATION TESTS

GC-MS Spectrum:

METHOD: G.C-MS conditions:

Column: Agilent Technologies, Elite -5MS, 30 m X 0.25 mm, 1.0micron

Instrument: Perkin Elmer, Carrier gas: Helium

Source Temp.: 230°C, Transfer line: 250°C

Inlet Temp.: 180°C, Diluent: Methanol

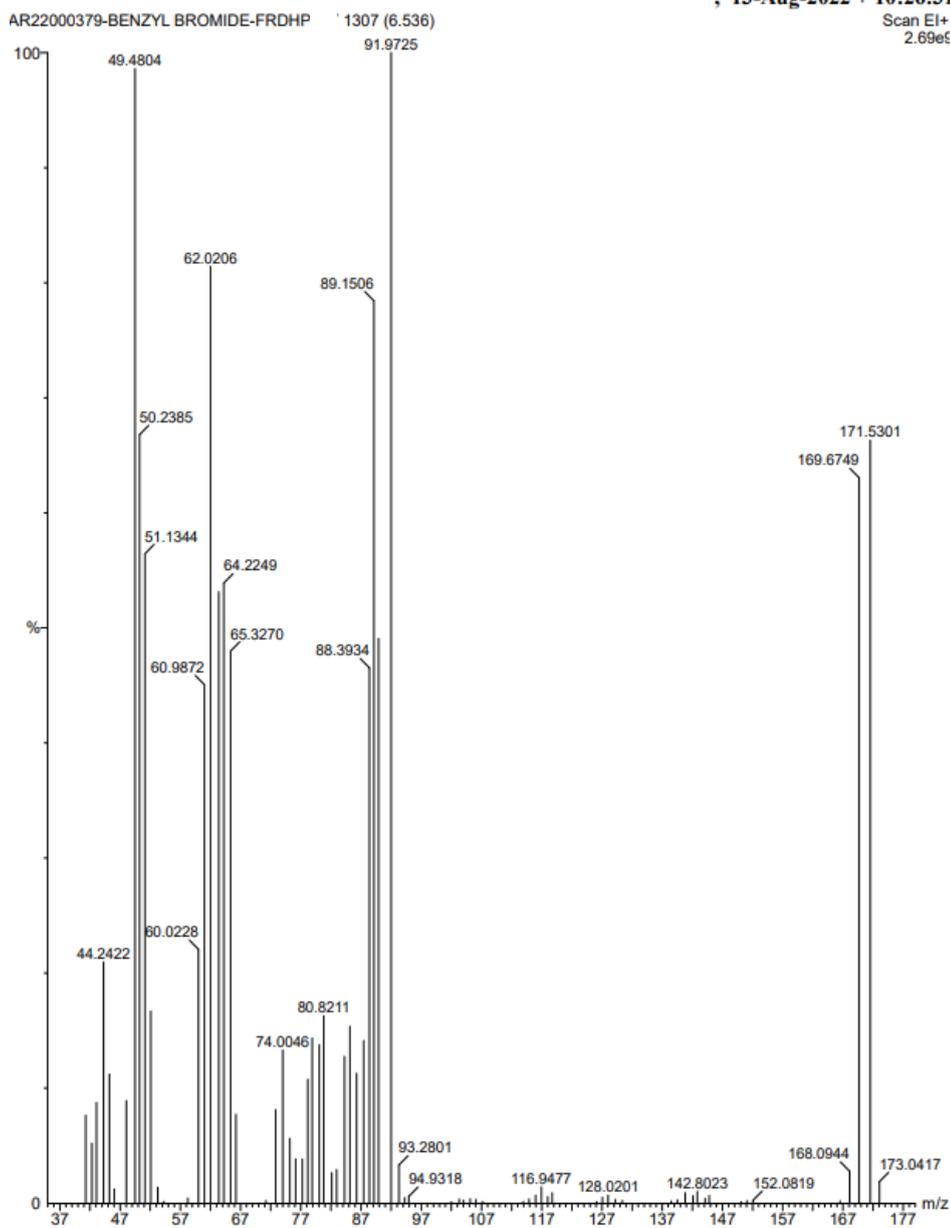
Source energy: 70eV

Mass by GC-MS:

Product Name: Benzyl bromide

Product Code: PSI132

, 13-Aug-2022 + 10:26:31



Identification by GC-MS: Conforms to molecular mass

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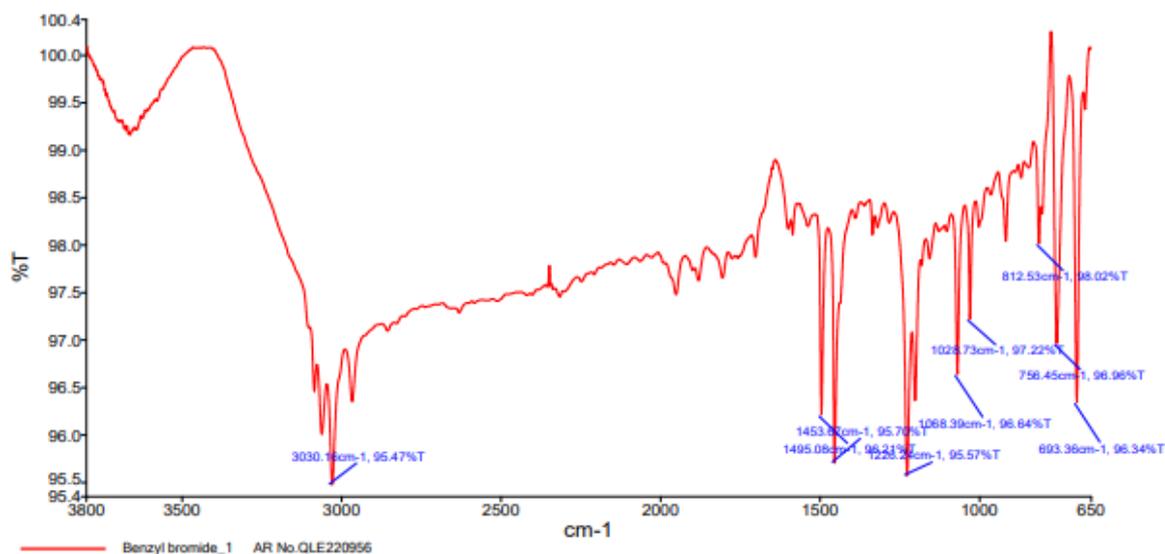
Infrared spectrum:

Product Name: Benzyl bromide

Product Code: PSI132

PerkinElmer Spectrum IR ES Version 10.6.1
18 August 2022 13:36

Analyst
Date



Source Spectra Results	
Spectrum Name	Number Of Peaks
Benzyl bromide_1	9

List of Peak Area/Height		
Peak Number	X (cm-1)	Y (%T)
1	3030.16	95.47
2	1495.08	96.21
3	1453.67	95.70
4	1226.24	95.57
5	1068.39	96.64
6	1028.73	97.22
7	812.53	98.02
8	756.45	96.96
9	693.36	96.34

Identification by IR: Conforms to structure

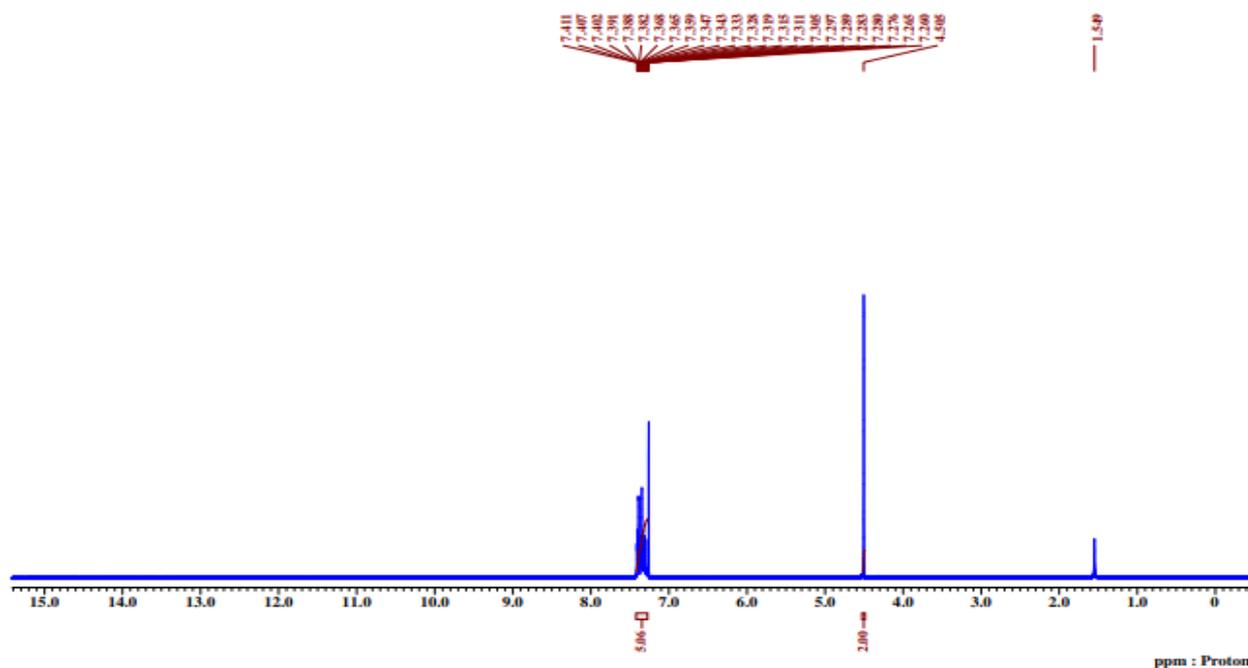
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¹H NMR Spectrum:

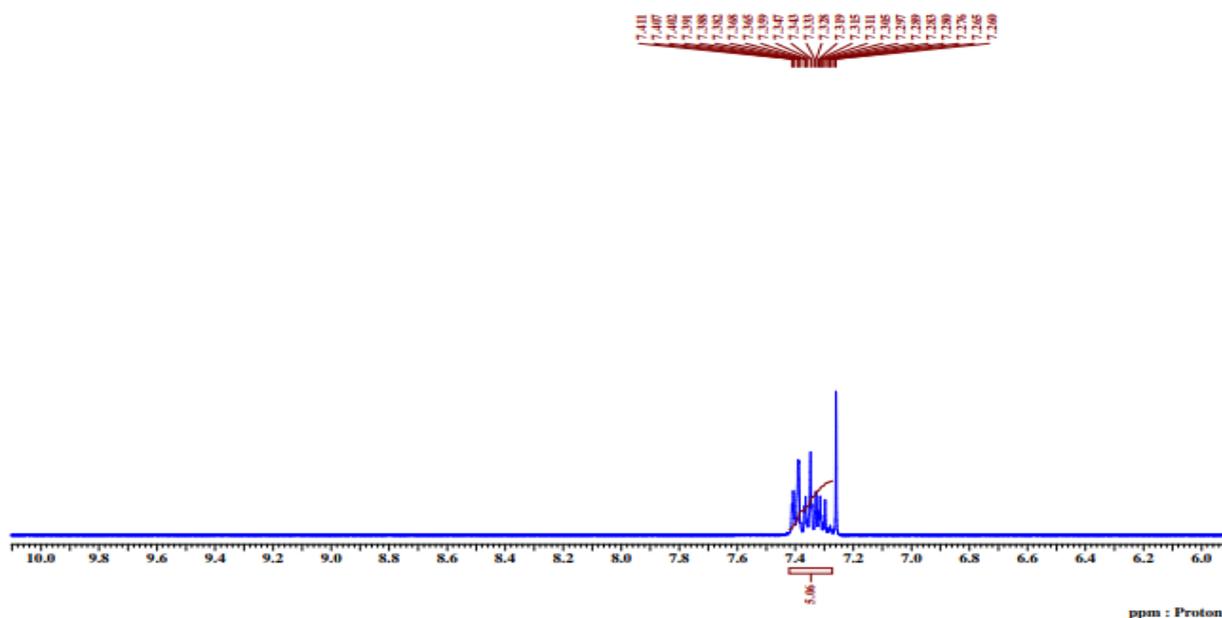
Product Name: Benzyl bromide

Product Code: PSI132



Sample_Id = Benzyl bromide-FRDND	Experiment = proton.jxp	Relaxation_Delay = 5[s]
Author = delta	X_Domain = Proto	Exp_Total = 205.0[s]
Creation_Time = 18-AUG-2022 18:07:04	Dir_Title = Proton	
Revision_Time = 18-AUG-2022 18:52:28	Solvent = CHLOROFORM-D	
Experiment_Details = JEGG[Delta VS.3.2]	Scans = 19	
Instrument = JNM-ECH400S/L1	Temp_Set = 18.8[$^{\circ}$ C]	
Spectrometer = JNM-ECH400S/L1	X_Acq_Time = 1.16916224[s]	

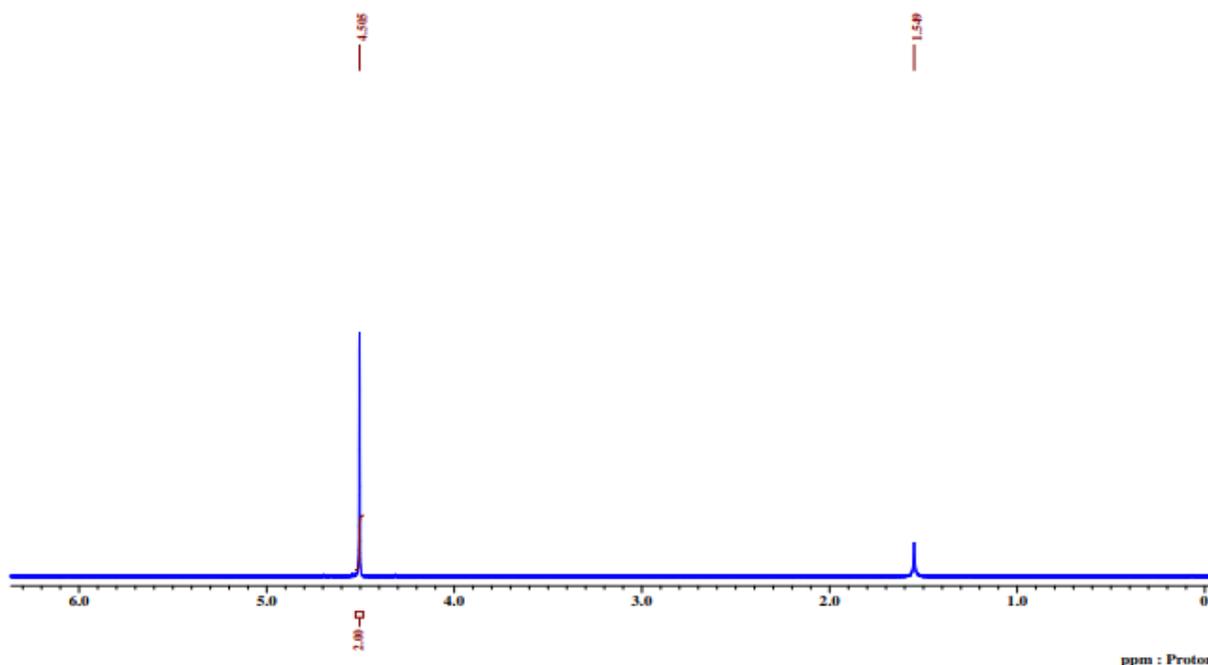
¹H NMR Spectrum: Expansion



Sample_Id = Benzyl bromide-FRDND	Experiment = proton.jxp	Relaxation_Delay = 5[s]
Author = delta	X_Domain = Proto	Exp_Total = 205.0[s]
Creation_Time = 18-AUG-2022 18:07:04	Dir_Title = Proton	
Revision_Time = 18-AUG-2022 18:52:28	Solvent = CHLOROFORM-D	
Experiment_Details = JEGG[Delta VS.3.2]	Scans = 19	
Instrument = JNM-ECH400S/L1	Temp_Set = 18.8[$^{\circ}$ C]	
Spectrometer = JNM-ECH400S/L1	X_Acq_Time = 1.16916224[s]	

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Sample_Id	= Benzyl bromide-FRDMF	Experiment	= proton_jkp	Relaxation_Delay	= 5[s]
Author	= delta	K_Domain	= Proto	Exp_Total	= 205.0[s]
Creation_Time	= 18-AUG-2022 18:07:04	Dir_Name	= Proton		
Revision_Time	= 18-AUG-2022 18:52:28	Solvent	= CHLOROFORM-D		
Experiment Details		Scans	= 19		
Instrument	= JEOL[Delta VS 3 2]	Temp_Set	= 18.8[°C]		
Spectrometer	= JNM-ECZ400S/1L	X_Acq_Time	= 1.16916224[s]		

Identification by ¹H NMR: Conforms to structure

Maximum limits of impurities

WATER DETERMINATION

Method: Karl Fisher titration

Water Content (PSI132) = **0.0923 %**

Approved By
Head - Technical

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