

# Certificate of Analysis

## 3-Pentanone

### PurCert Standard for GC

<b>Product Number</b>	PSR28335	<b>CAS No.</b>	96-22-0
<b>Brand</b>	PureSynth	<b>Lot No.</b>	TEJ05H
<b>Molecular Formula</b>	C <sub>5</sub> H <sub>10</sub> O	<b>Date of Mfg.</b>	May,2021
<b>Molecular Weight</b>	86.13 g/mol	<b>Date of Exp.</b>	April,2025

Test	Specification	Result
Description	Colorless liquid	Colorless liquid
Clarity	Clear	Clear
Assay (GC-FID)	≥ 99.5 %	99.69%
Water (by KF)	≤ 0.05%	0.045 %
Identification by <sup>1</sup> H NMR	Conform to structure	Conforms
Identification by GC-MS	Conform to molecular	Conforms
Identification by IR	Conform to structure	Conforms

**\*Traceable to Internal Reference standard.**

**Storage Condition:** Store at ambient temperature and keep container tightly closed in a dry and well-Ventilated place.

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

*This is a computer-generated report -does not required sign*

Worldwide Helpline No. 1800-120-1234-34 , Email: [info@pure-synth.com](mailto:info@pure-synth.com) , Website: [www.pure-synth.com](http://www.pure-synth.com)

## Assay by GC-FID

### METHOD: G.C- FID conditions:

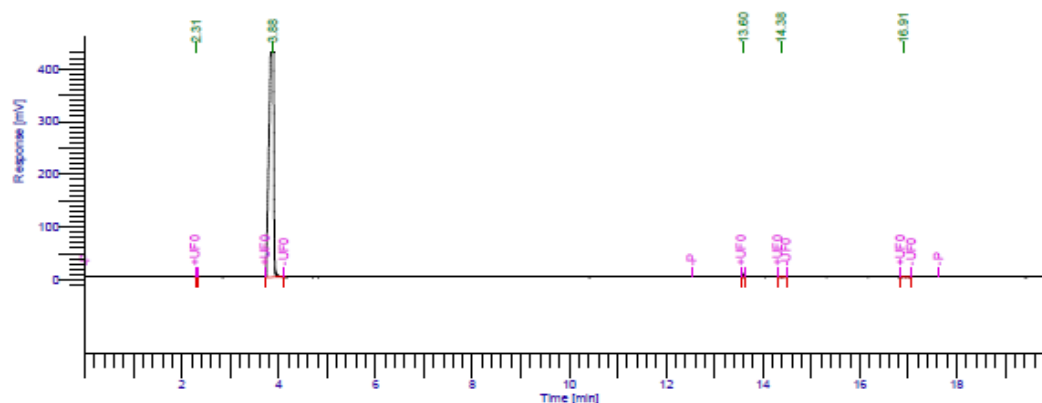
**Column:** Agilent Technologies DB-FFAP 30mx 0.530mm, 1.0micron

**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	: 03-07-2021 4.36.05 PM
Operator	: manager	Sample Name	: AR21000379_1-3-PENTANONE- TEJ
Sample Number	: 1		: 05H
AutoSampler	: BUILT-IN		
Instrument Name	: Clarus 680	Study	: GC Purity
Instrument Serial #	: None	Rack/Vial	: 0/4
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	: 20.00 min
Sample Amount	: 1.0000		
Data Acquisition Time	: 03-07-2021 9.34.41 AM	Area Reject	: 0.000000
		Dilution Factor	: 1.00
		Cycle	: 1



### GC Reports

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]
1		2.308	413.74	252.26	0.01
2		3.881	3476084.74	640604.32	99.69
3		13.597	8895.36	5695.61	0.26
4		14.384	546.28	239.57	0.02
5		16.907	803.67	138.25	0.02
			3486743.78	646930.01	100.00

#### Missing Component Report

Component Expected Retention (Calibration File)

All components were found

**Purity by GC-FID: 99.69 %**

*This is a computer-generated report -does not required sign*

Worldwide Helpline No. 1800-120-1234-34 , Email: [info@pure-synth.com](mailto:info@pure-synth.com) , Website: [www.pure-synth.com](http://www.pure-synth.com)

## 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

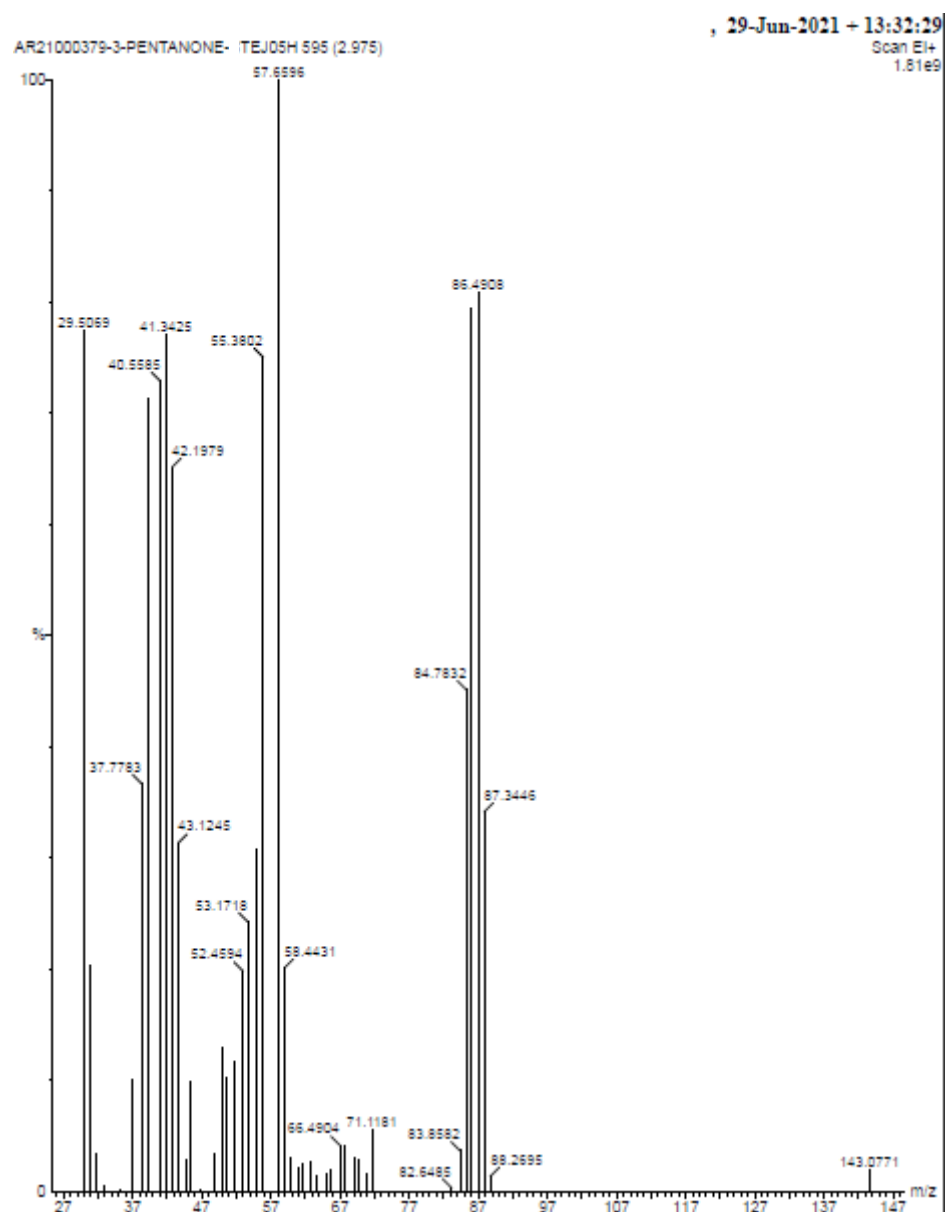
**Inlet Temp.:** 180°C, **Diluent:** Methanol

**Source energy:** 70eV

### Mass by GC-MS:

**Product Name:** 3-Pentanone

**Product Code:** PSR28335



**Identification by GC-MS: Conform to molecular**

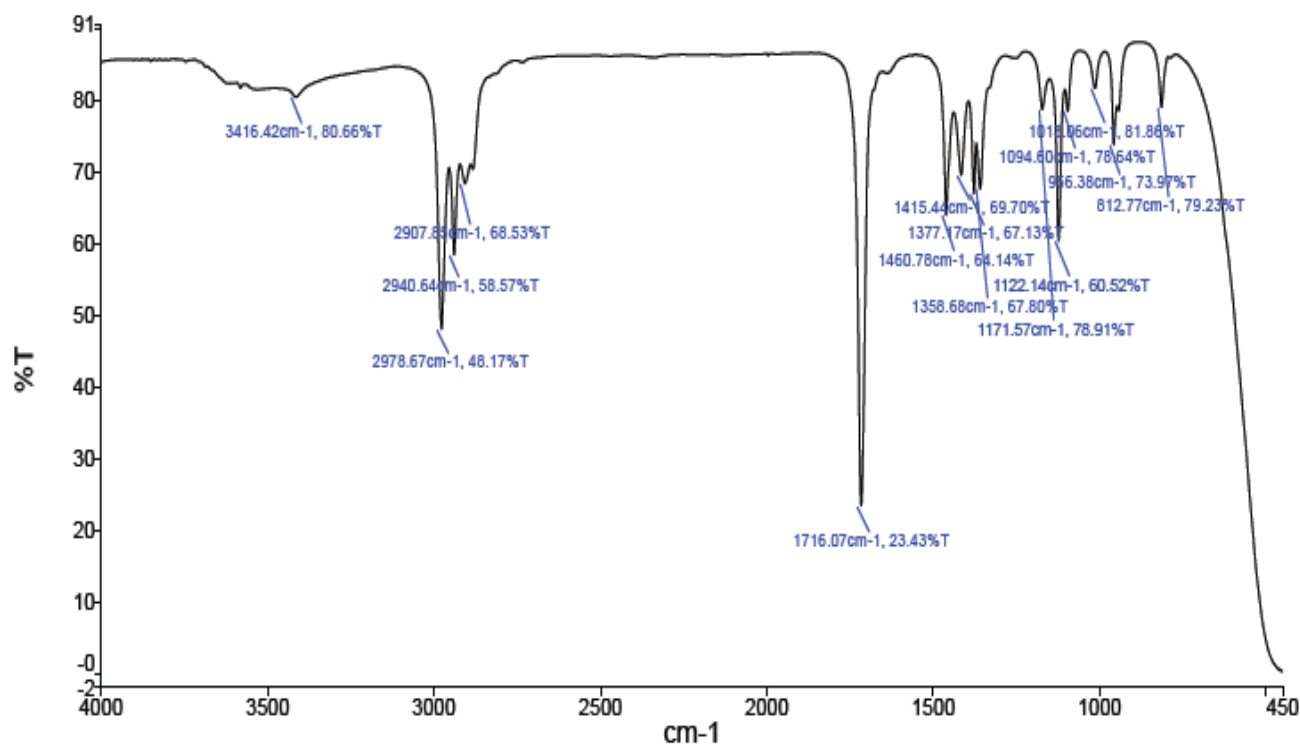
*This is a computer-generated report -does not required sign*

**Worldwide Helpline No.** 1800-120-1234-34 , Email: [info@pure-synth.com](mailto:info@pure-synth.com) , Website: [www.pure-synth.com](http://www.pure-synth.com)

# *Infrared spectrum:*

**Product Name: 3-Pentanone**

**Product Code: PSR28335**



Source Spectra Results	
Spectrum Name	Number Of Peaks
3-Pentanone	15

List of Peak Area/Height		
Peak Number	X (cm-1)	Y (%T)
1	3416.42	80.66
2	2978.67	48.17
3	2940.64	58.57
4	2907.85	68.53
5	1716.07	23.43
6	1460.78	64.14
7	1415.44	69.70
8	1377.17	67.13
9	1358.68	67.80
10	1171.57	78.91
11	1122.14	60.52
12	1094.60	78.64
13	1013.06	81.86
14	956.38	73.97
15	812.77	79.23

**Identification by IR: Conform to structure**

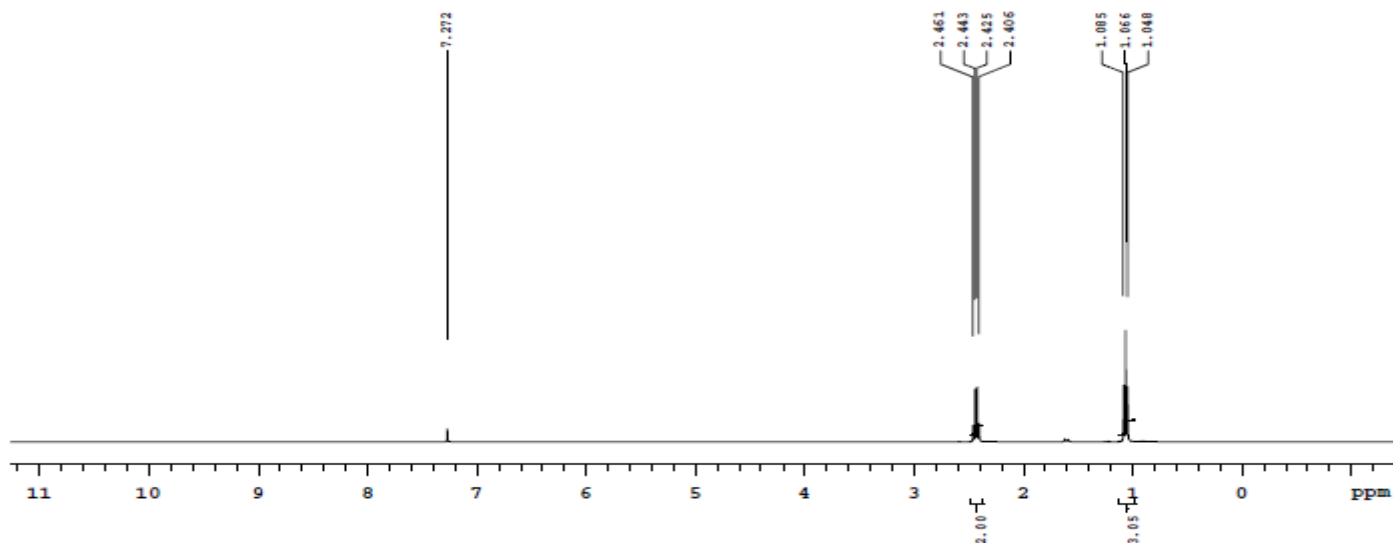
*This is a computer-generated report -does not required sign*

Worldwide Helpline No. 1800-120-1234-34 , Email: [info@pure-synth.com](mailto:info@pure-synth.com) , Website: [www.pure-synth.com](http://www.pure-synth.com)

# <sup>1</sup>H NMR Spectrum:

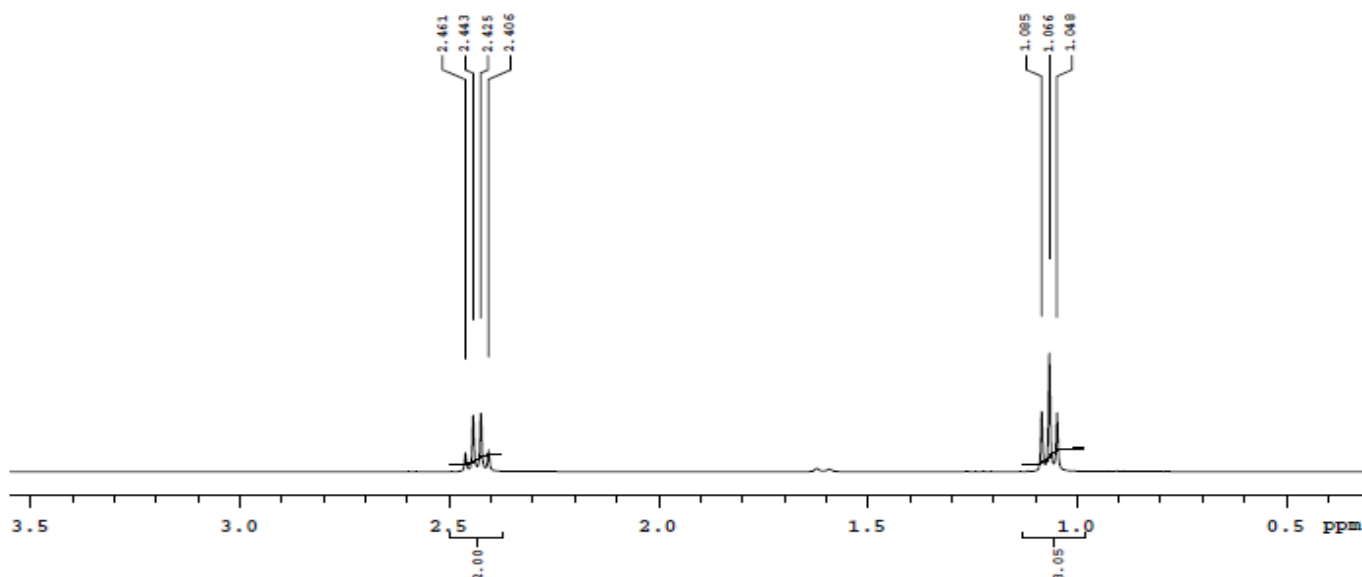
Product Name: 3-Pentanone

Product Code: PSR28335



<b>PULSE SEQUENCE</b> Relax. delay 2.000 sec Pulse 45.0 degrees Acq. time 3.408 sec Width 9615.4 Hz 16 repetitions	<b>OBSERVE</b> H1, 399.8212849	<b>DATA PROCESSING</b> Line broadening 1.0 Hz FT size 65536 Total time 1 minute	<b>3-Pentanone-1H</b> TEJ05H Solvent: cdcl3 Ambient temperature Operator: vnmr1 VNMRS-400 "Agilent-NMR"
---	--------------------------------	--	--

## <sup>1</sup>H NMR Spectrum: Expansion



<b>PULSE SEQUENCE</b> Relax. delay 2.000 sec Pulse 45.0 degrees Acq. time 3.408 sec Width 9615.4 Hz 16 repetitions	<b>OBSERVE</b> H1, 399.8212849	<b>DATA PROCESSING</b> Line broadening 1.0 Hz FT size 65536 Total time 1 minute	<b>3-Pentanone-1H</b> TEJ05H Solvent: cdcl3 Ambient temperature Operator: vnmr1 VNMRS-400 "Agilent-NMR"
---	--------------------------------	--	--

Identification by 1H NMR: Conform to structure

*This is a computer-generated report -does not required sign*

Worldwide Helpline No. 1800-120-1234-34 , Email: [info@pure-synth.com](mailto:info@pure-synth.com) , Website: [www.pure-synth.com](http://www.pure-synth.com)

## Maximum limits of impurities

---

### WATER DETERMINATION

Method: Karl Fisher titration

Water Content (PSR28335) = **0.045%**

Approved By  
Head - Technical

---

*This is a computer-generated report -does not required sign*

Worldwide Helpline No. 1800-120-1234-34 , Email: [info@pure-synth.com](mailto:info@pure-synth.com) , Website: [www.pure-synth.com](http://www.pure-synth.com)