

Certificate of Analysis

4-Phenylbut-3-en-2-one

PurCert Standard for GC

Product Number	PSR42119	CAS No.	122-57-6
Brand	PureSynth	Lot No.	P42119B0923
Molecular Formula	C ₁₀ H ₁₀ O	Date of Mfg.	September.2023
Molecular Weight	146.19 g/mol	Date of Exp.	August.2027

Test	Specification	Result
Description	Pale-yellow Solid	Pale-yellow Solid
Assay (GC-FID)	≥ 98.0 %	98.14 %
Water (By KF)	NMT 0.2000 %	0.1415 %
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 the container tightly closed.

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

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Assay by GC-FID

METHOD: GC- FID conditions:

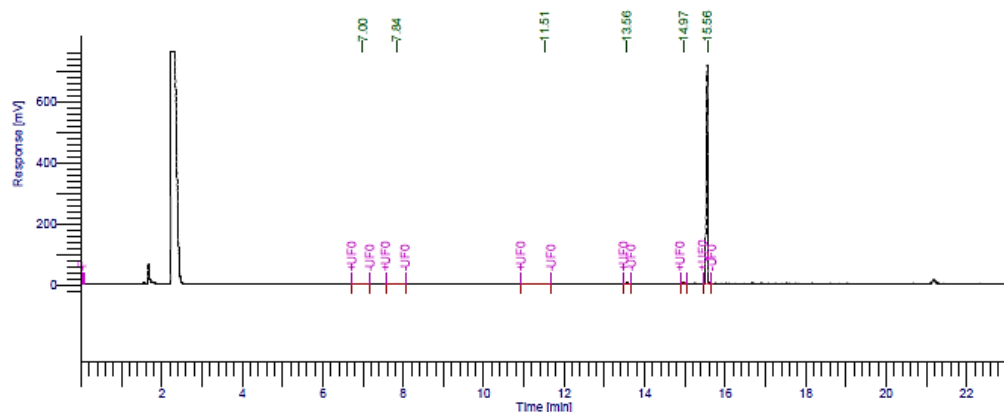
Column: Agilent Technologies DB-FFAP 30mx 0.530mm, 1.0micron

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 : 05-12-2023 17:34:41
Operator : manager	Sample Name : 4-PHENYL BUT-3EN-2ONE-P42119B0
Sample Number : 001	923
AutoSampler : BUILT-IN	
Instrument Name : Clarus 690	Study :
Instrument Serial # : None	Rack/Vial : 0/45
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 : 23.00 min
Sample Amount : 1.0000	
Data Acquisition Time : 05-12-2023 11:50:19	Area Reject : 0.000000
	Dilution Factor : 1.00
	Cycle : 1



GC Reports

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]
1		6.995	5533.41	705.22	0.31
2		7.839	3274.81	518.23	0.18
3		11.511	10276.64	554.57	0.57
4		13.556	7199.14	2240.54	0.40
5		14.968	6930.21	3362.89	0.39
6		15.559	1755985.30	715919.33	98.14
			1789199.51	723300.78	100.00

Missing Component Report
Component Expected Retention (Calibration File)

All components were found

Purity by GC-FID: 98.14 %

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IDENTIFICATION TESTS

GC-MS Spectrum:

METHOD: GC-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:

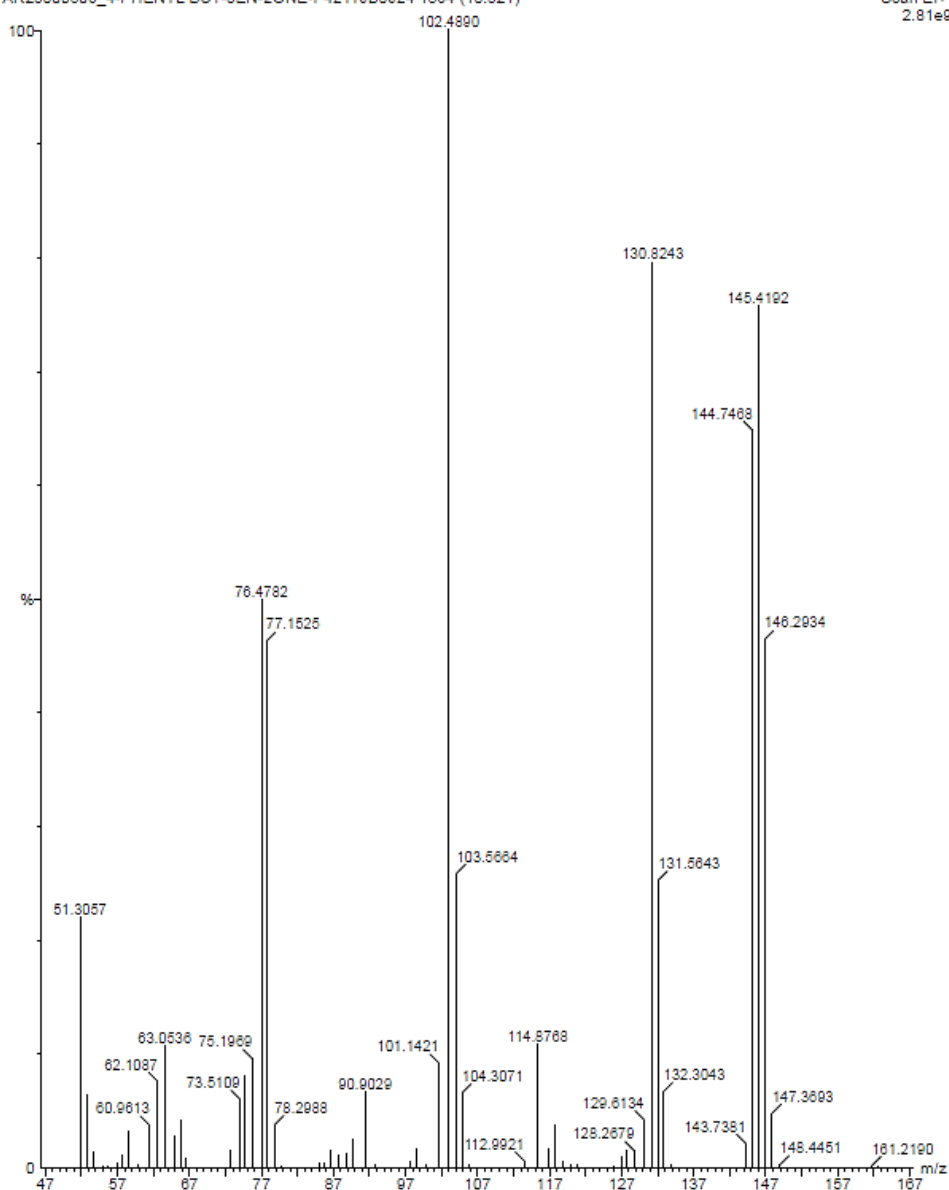
Product Name: 4-Phenylbut-3-en-2-one

Product Code: PSR42119

, 05-Dec-2023 + 11:40:16

AR23000806_4-PHENYL BUT-3EN-2ONE-P42119B0924 1364 (10.321)

Scan EI+
2.81e9



Identification by GC-MS: Conforms to molecular mass

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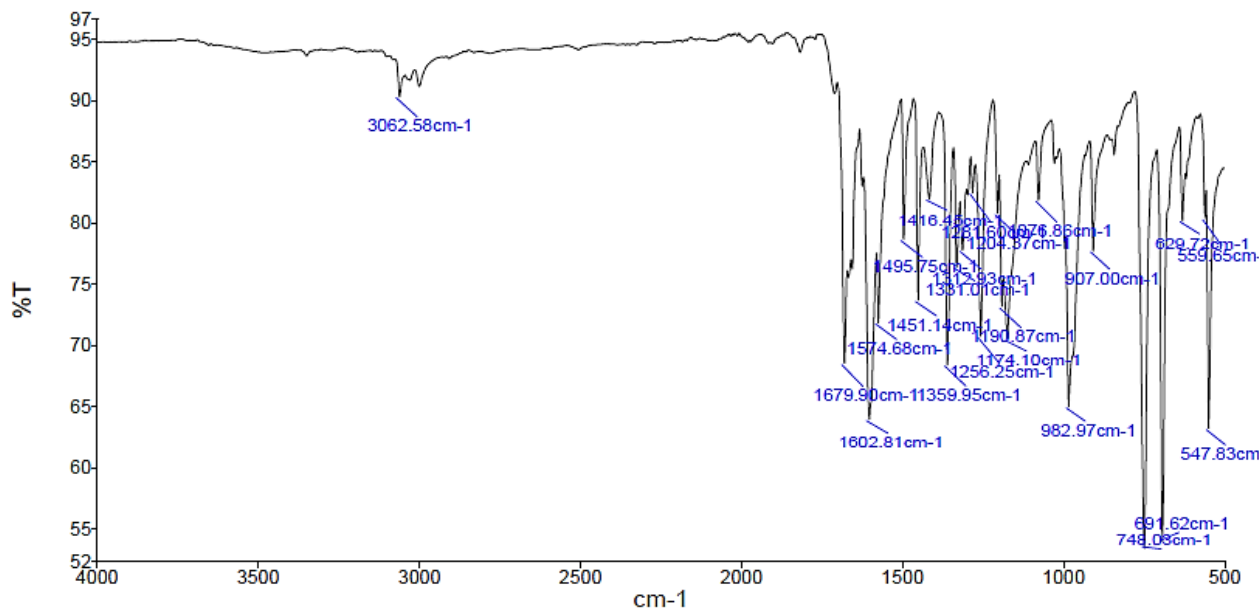
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Infrared spectrum:

Product Name: 4-Phenylbut-3-en-2-one

Product Code: PSR42119

Analyst
Date



AR23000164- 4-Phenylbut-3-en-2-one-P42119B0923_1 Sample 002 By Analyst Date Tuesday, December 05 2023

Source Spectra Results		
Spectrum Name	Number Of Peaks	
AR23000164- 4-Phenylbut-3-en-2-one-P42119B0923_1	23	
List of Peak Area/Height		
Peak Number	X (cm-1)	Y (%T)
1	3062.58	90.33
2	1679.90	68.54
3	1602.81	63.96
4	1574.68	71.87
5	1495.75	78.66
6	1451.14	73.70
7	1416.45	81.97
8	1359.95	68.43
9	1331.01	76.41
10	1312.93	77.80
11	1281.60	82.49
12	1256.25	70.76
13	1204.37	80.80
14	1190.87	73.18
15	1174.10	70.53
16	1076.86	81.90
17	982.97	65.01
18	907.00	77.73
19	748.03	53.39
20	691.62	53.96
21	629.72	80.20
22	559.65	80.39
23	547.83	63.21

Identification by IR: Conforms to structure

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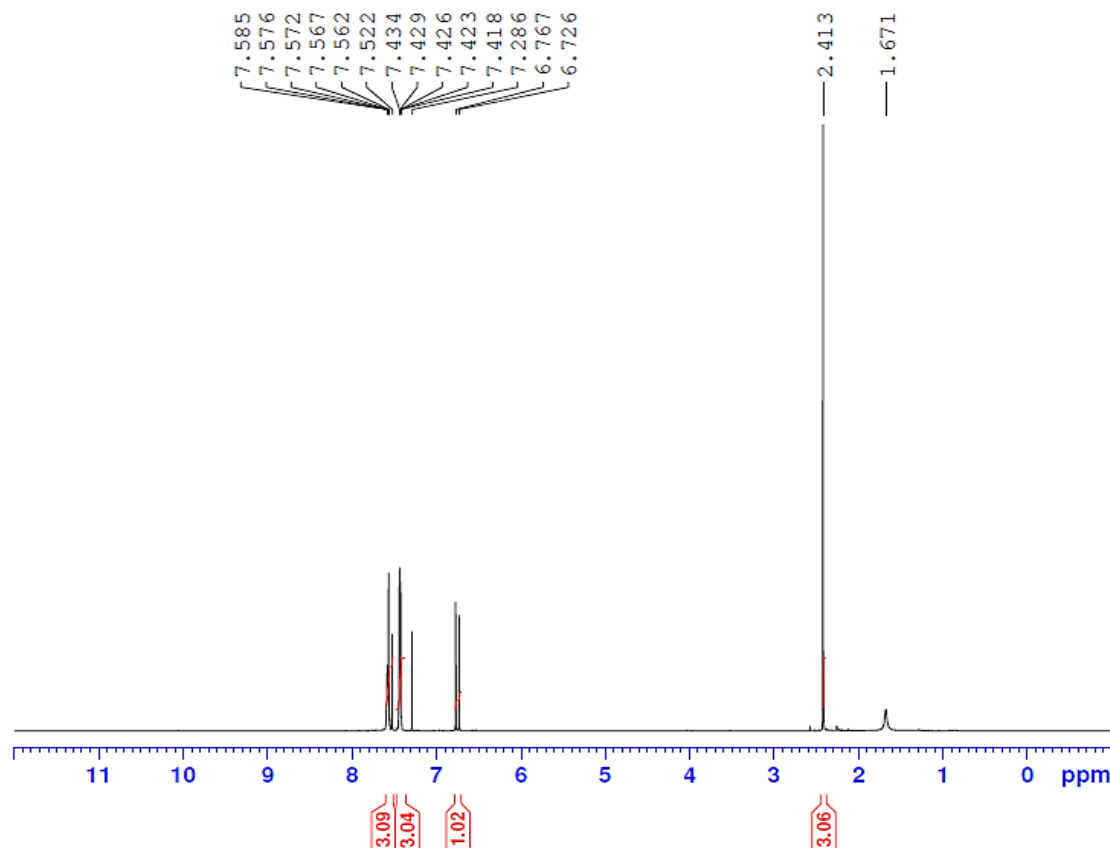
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¹H NMR Spectrum:

Product Name: 4-Phenylbut-3-en-2-one

Product Code: PSR42119

4-Phenylbut-3-en-2-one
B.no-P42119B0923
1H-NMR in CDCl₃



Identification by ¹H NMR: Conforms to structure

Maximum limits of impurities

WATER DETERMINATION

Method: Karl Fisher titration

Water Content (PSR42119) = **0.1415 %**

Approved By
Head - Technical

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