

# Certificate of Analysis

## Caffeine

### PurCert Standard

<b>Product Number</b>	PSR37982	<b>CAS No.</b>	58-08-2
<b>Brand</b>	PureSynth	<b>Lot No.</b>	GFH12IT
<b>Molecular Formula</b>	C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>	<b>Date of Mfg.</b>	Dec.2021
<b>Molecular Weight</b>	194.19 g/mol	<b>Date of Exp.</b>	Nov.2024

Test	Specification	Result
Description	White powder	White powder
Assay (HPLC)	≥99.5%	99.976%
Water (by KF)	≤0.3%	0.2721%
Identification by GC-MS	Conform to molecular	Conforms
Identification by <sup>1</sup> H NMR	Conform to structure	Conforms
Identification by IR	Conform to structure	Conforms

**\*Traceable to USP Reference Standard 1085003, lot no: R04330.**

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

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

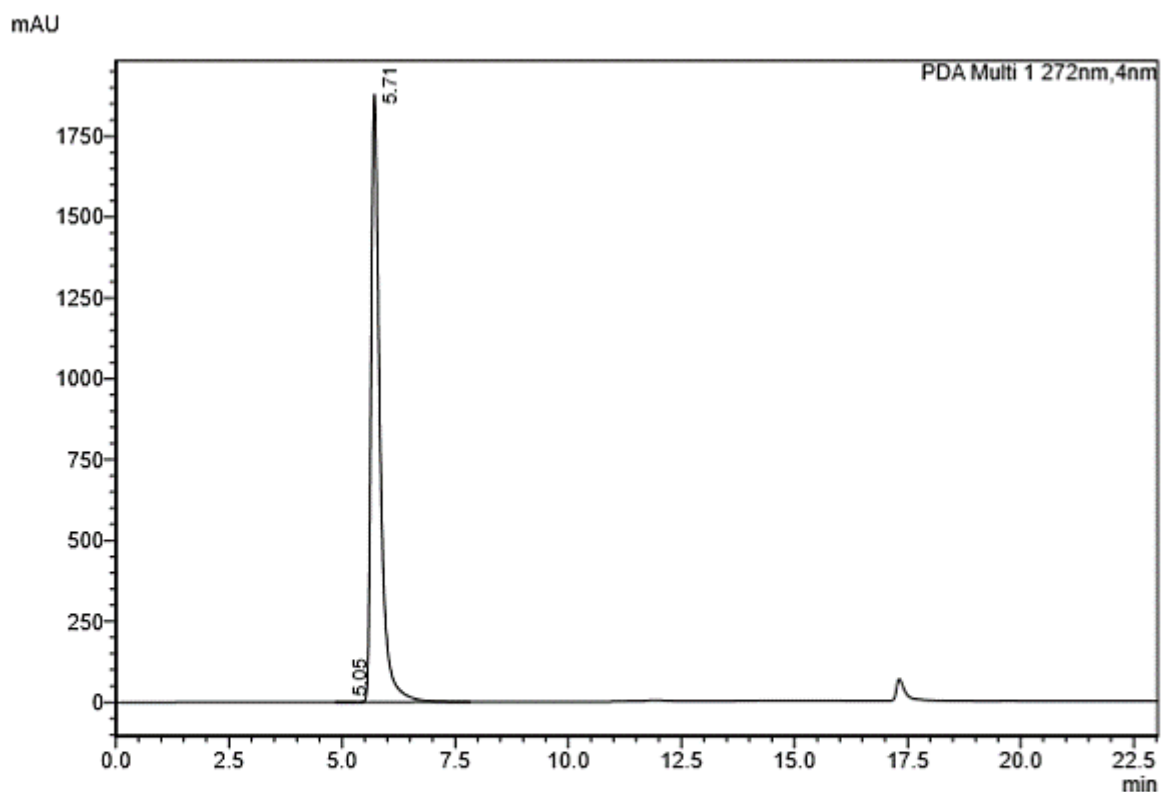
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## Assay by HPLC

### Chromatogram



### Peak Table

PDA Ch1 272nm

Peak#	Ret. Time	Area	Area%
1	5.05	6173	0.024
2	5.71	25872428	99.976
Total		25878601	100.000

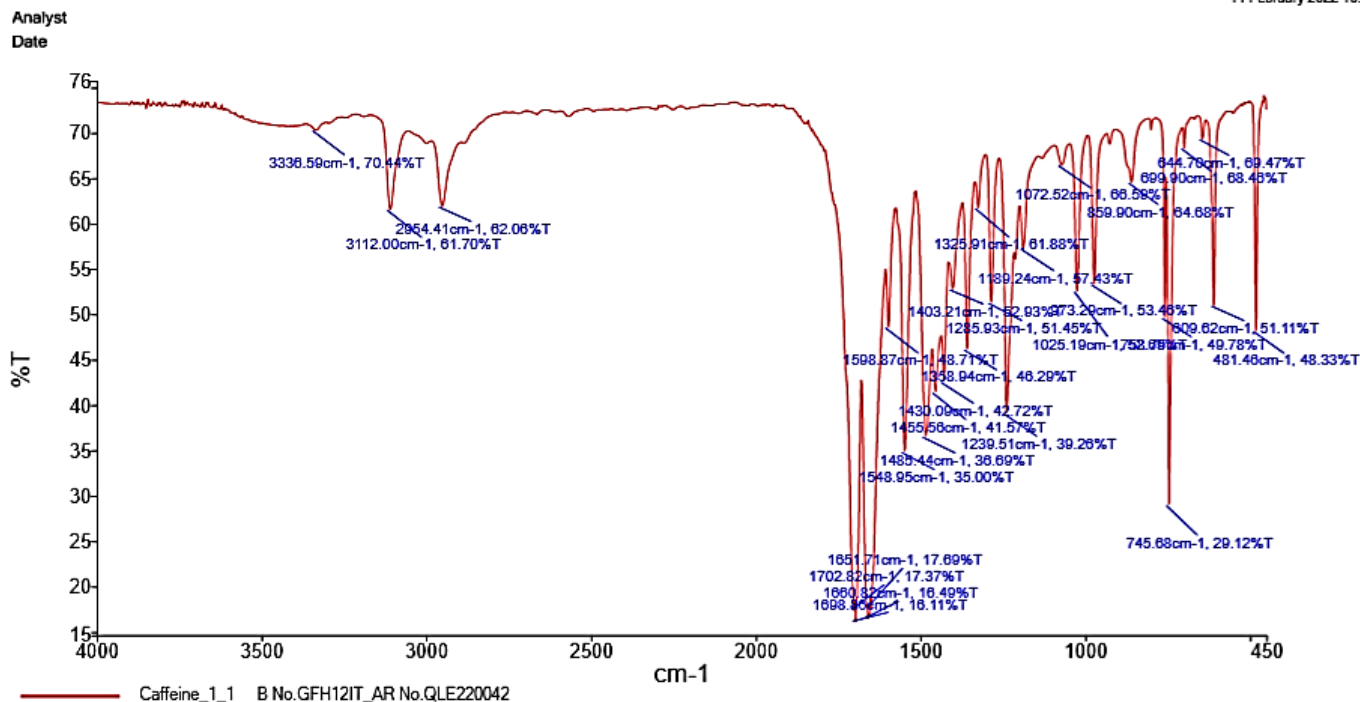
**Purity by HPLC: 99.976%**

**Infrared spectrum:**

**Product Name: Caffeine**

**Product Code: PSR37982**

PerkinElmer Spectrum IR ES Version 10.6.1  
14 February 2022 15:47



**Source Spectra Results**

Spectrum Name	Number Of Peaks
Caffeine_1_1	28

PerkinElmer Spectrum IR ES Version 10.6.1  
14 February 2022 15:47

**List of Peak Area/Height**

Peak Number	X (cm-1)	Y (%T)
1	3336.59	70.44
2	3112.00	61.70
3	2954.41	62.06
4	1702.82	17.37
5	1698.86	16.11
6	1660.82	16.49
7	1651.71	17.69
8	1598.87	48.71
9	1548.95	35.00
10	1485.44	36.69
11	1455.56	41.57
12	1430.09	42.72
13	1403.21	52.93
14	1358.94	46.29
15	1325.91	61.88
16	1285.93	51.45
17	1239.51	39.26
18	1189.24	57.43
19	1072.52	66.59
20	1025.19	52.69
21	973.29	53.46
22	859.90	64.68
23	758.75	49.78
24	745.68	29.12
25	699.90	68.46
26	644.70	69.47
27	609.62	51.11
28	481.46	48.33

**Identification by IR: Conform to structure**

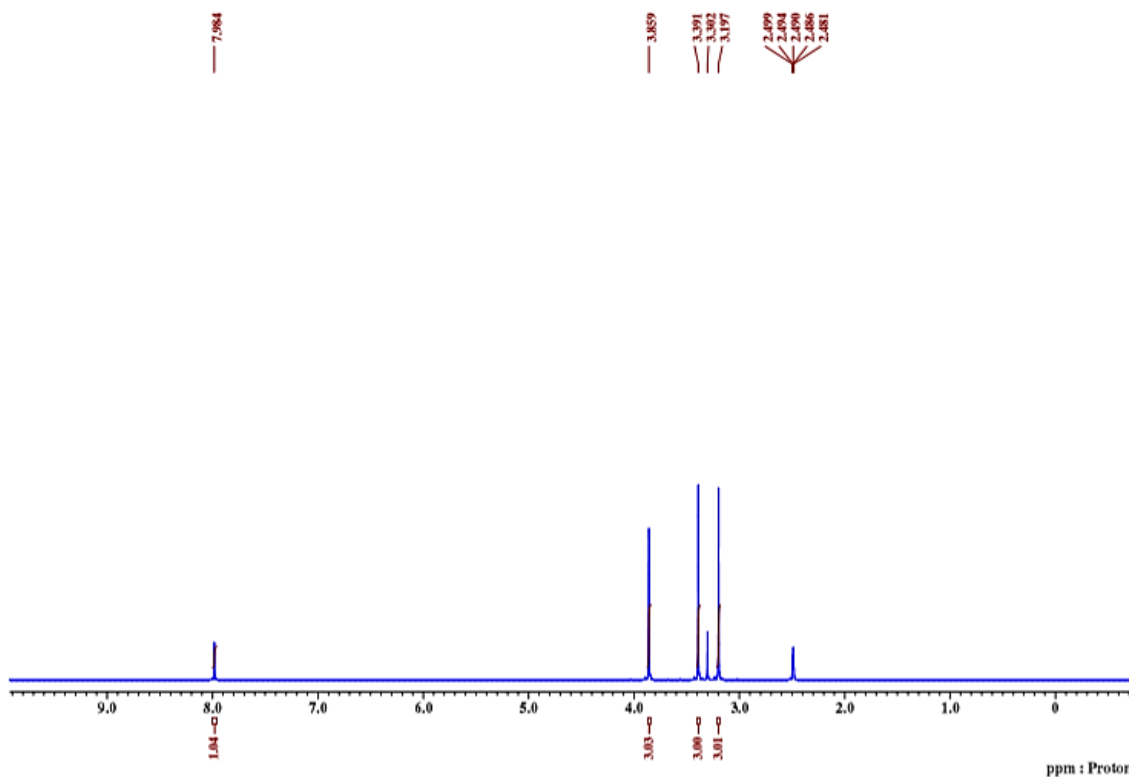
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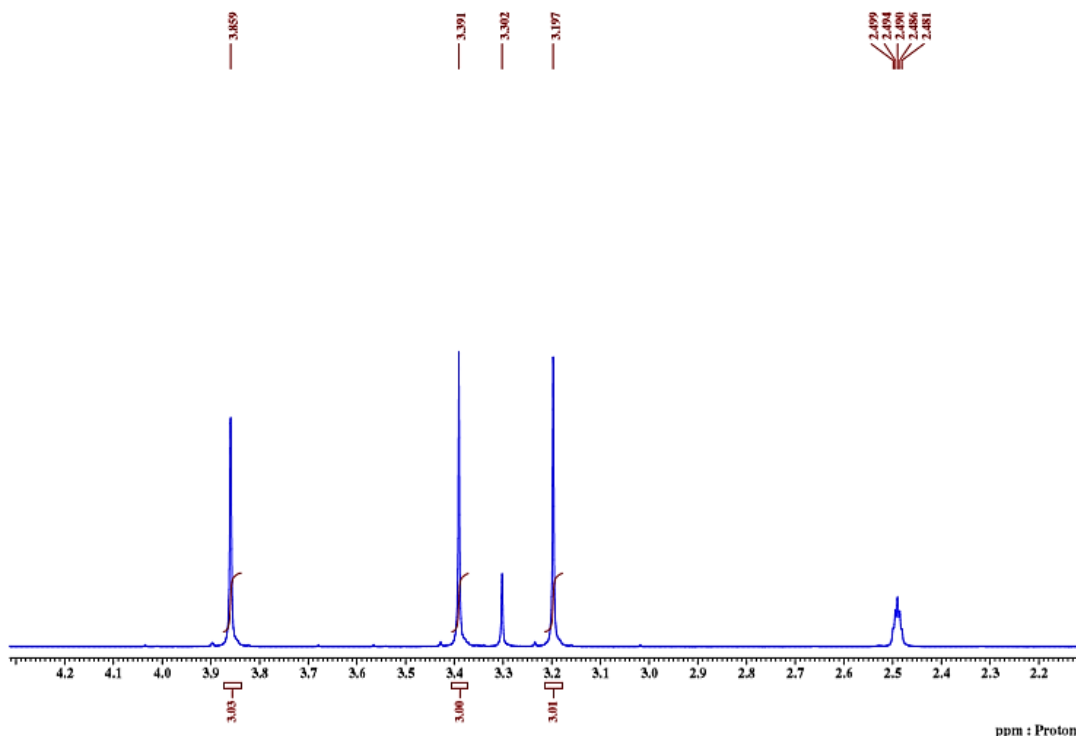
**<sup>1</sup>H NMR Spectrum:**

**Product Name: Caffeine**

**Product Code: PSR37982**



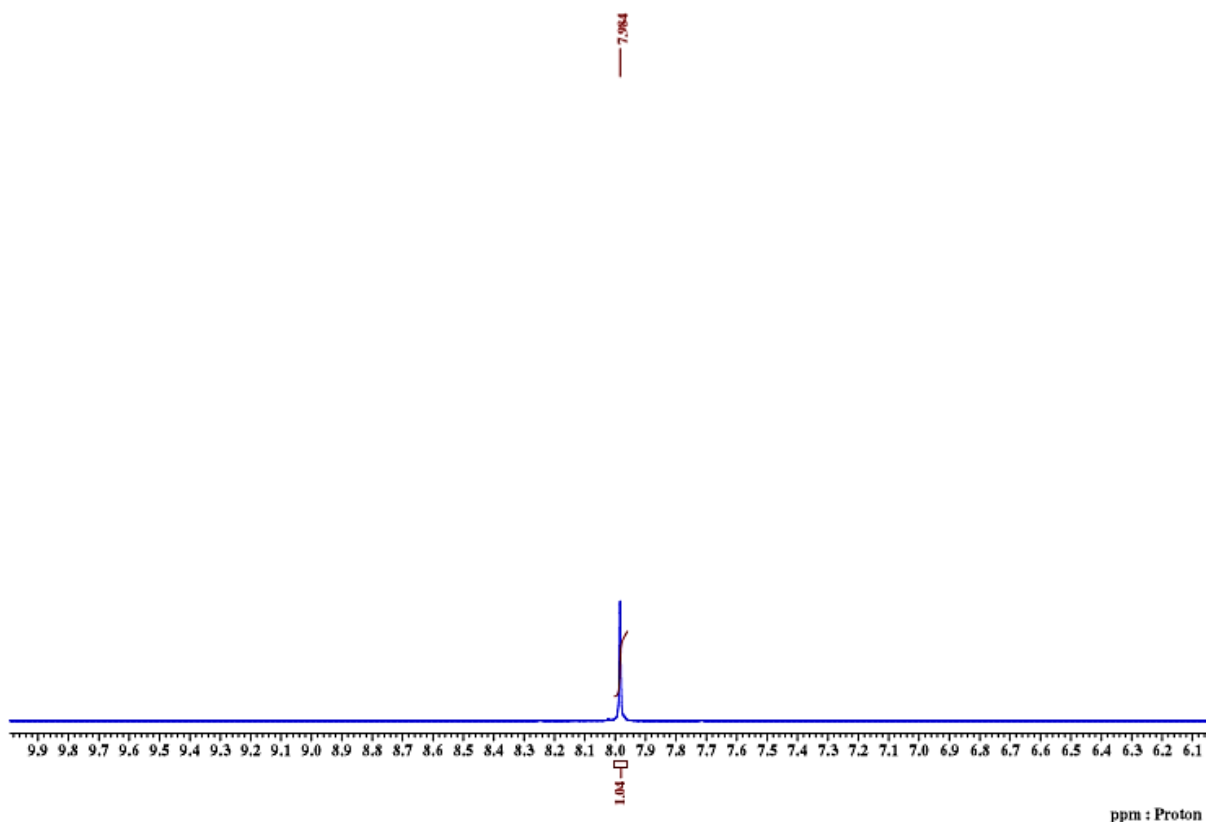
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 Revision\_Time = 17-FEB-2022 10:38:43 Solvent = DMSO-D6  
 Experiment Details Scans = 23  
 Instrument = JBO1(Delta VS J.2) Temp\_Set = 25[degC]  
 Spectrometer = JNM-ECZ400S/L1 X\_Acq\_Time = 1.16914224[s]



Sample\_Id = Caffeine Experiment = proton.jpg Relaxation\_Delay = 3[s]  
 Author = delta X\_Domain = Proton Exp\_Total = 205.0[s]  
 Creation\_Time = 17-FEB-2022 10:33:24 Dir\_File = Proton  
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 Experiment Details Scans = 23  
 Instrument = JBO1(Delta VS J.2) Temp\_Set = 25[degC]  
 Spectrometer = JNM-ECZ400S/L1 X\_Acq\_Time = 1.16914224[s]

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ppm : Proton

Sample_Id	= Caffeine	Experiment	= proton.jsp	Relaxation_Delay	= 5[s]
Author	= delta	X_Domain	= Proton	Exp_Total	= 205.0[s]
Creation_Time	= 17-FEB-2022 10:35:24	Dir_Title	= Proton		
Revision_Time	= 17-FEB-2022 10:38:43	Solvent	= CDCl3-D6		
Experiment_Details		Scans	= 23		
Instrument	= JNM-ECZ400S V5.3.2	Temp_Set	= 25[dc]		
Spectrometer	= JNM-ECZ400S/L1	X_Acq_Time	= 1.16916224[s]		

Identification by <sup>1</sup>H NMR: Conform to structure

## Maximum limits of impurities

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### WATER DETERMINATION

Method: Karl Fisher titration

Water Content (PSR37982) = **0.2721%**

Approved By  
Head - Technical

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