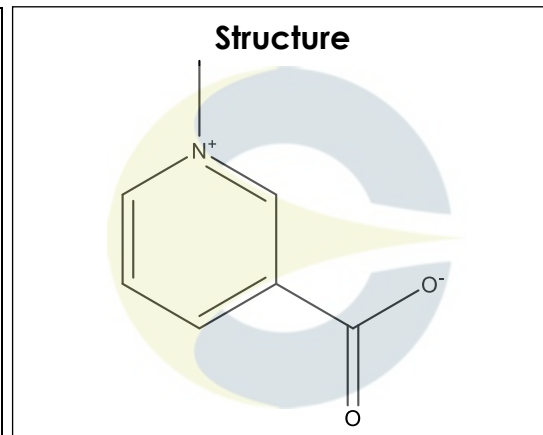


Certificate of Analysis

For Laboratory Use Only

PRODUCT NAME	Trigonelline
PART NUMBER	00020353
STANDARD TYPE	Primary (P)
LOT NUMBER	00020353-311
REPORT NUMBER	CDXA-RSS-10208-00
SAMPLE NUMBER	CHA203124
DATE OF SAMPLE	15May2023
DATE OF REPORT	27Jun2023



CHEMICAL NAMES	3-Carboxy-1-methyl-pyridinium inner salt; Betaine nicotinate; Caffeatine; N-Methylnicotinate
CHEMICAL FORMULA	C ₇ H ₇ NO ₂
MOLECULAR WEIGHT (MW)	137.14
CHEMICAL FAMILY	Alkaloids
CAS NUMBER	[535-83-1]
EC#(EINECS)	208-620-5
RTECS	YF6825000

ANALYTICAL RESULTS

TEST	METHOD	SPECIFICATION	RESULT
Adjusted Purity	NA	≥ 85%	91.1%
HPLC	0.700.10.2.METH3	≥ 90%	99.9%
NMR	0.700.12.4	Conforms to structure	Conforms to structure
Mass Spectrum	0.700.12.27	Conforms	Conforms
Residual Solvent*	USP <467>	NA	ND
Water	0.700.12.37	NA	8.8%
Appearance	NA	NA	White powder

*Testing performed at an ISO 17025 accredited subcontracted laboratory.

ADJUSTED PURITY: 91.1% IS BASED ON (100 - 0.0 SOLVENTS - 8.8 WATER) X 99.9% HPLC

STORAGE CONDITIONS

STORAGE	+4 °C in a dry place.
EXPIRATION DATE	05/2028 under the above conditions.

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ANALYTICAL CONDITIONS

INSTRUMENT AGILENT 1260 HPLC UV-VIS (DAD);
 AB-SCIEX 6600 TRIPLE TOF

COLUMN Se-quant ZIC-HILIC 150 x 4.6 mm, 5 µm particle size

MOBILE PHASE A – 2 mM ammonium formate, pH 3.9,
 B – 95:5 Acetonitrile: 2 mM ammonium formate, pH 3.9;

Minutes	%A	%B
0.0	0	100
5.0	0	100
25.0	45	55
29.9	45	55
30.0	0	100
38.0	0	100

COLUMN TEMP. 30 °C

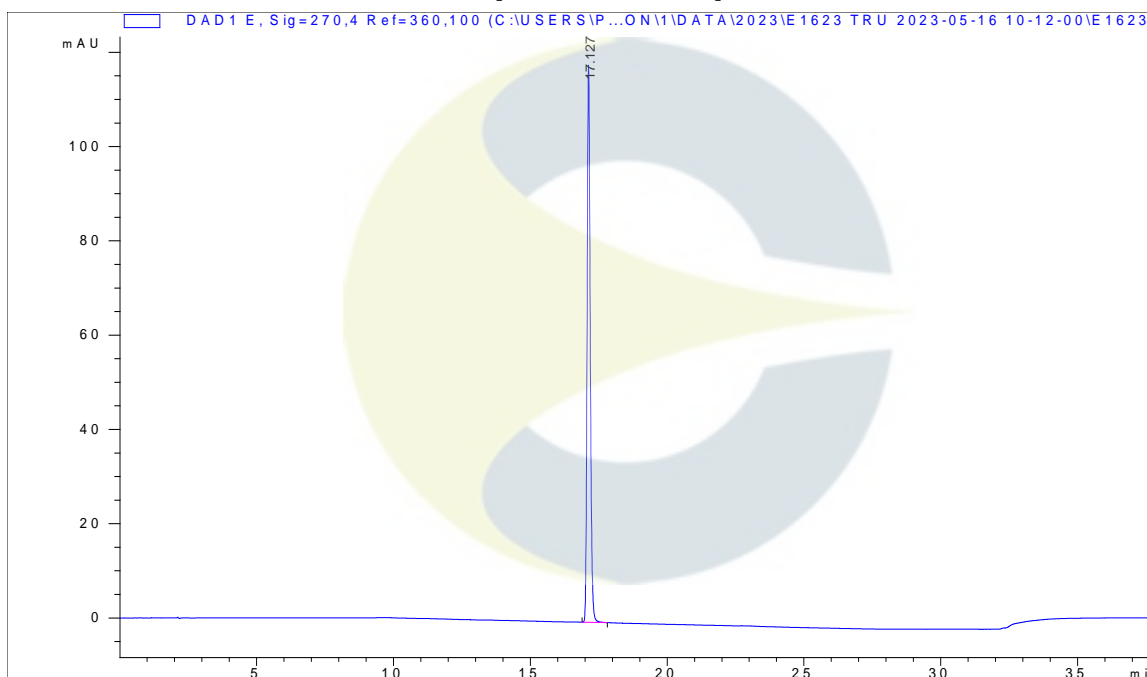
FLOW RATE 1.0 mL/minute

INJECTION VOL. 0.5 µL

INJECTION CONC. 1.3 mg/mL in Methanol

DETECTION 270 ± 2 nm

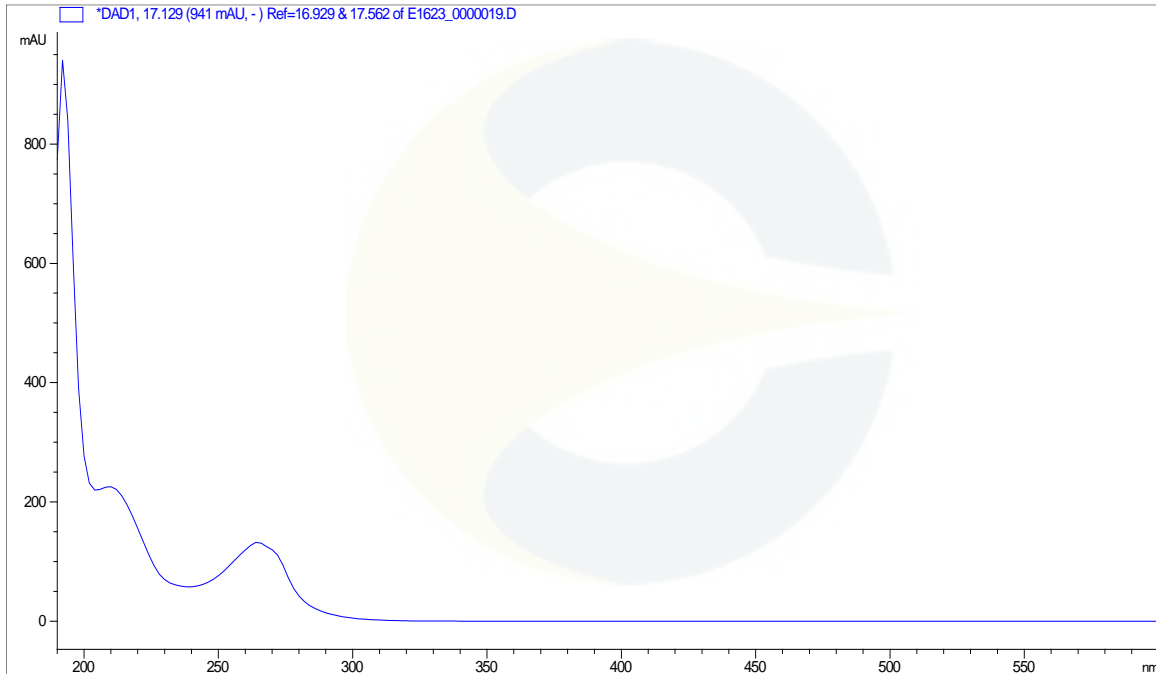
HPLC CHROMATOGRAM OF TRIGONELLINE (00020353-311)



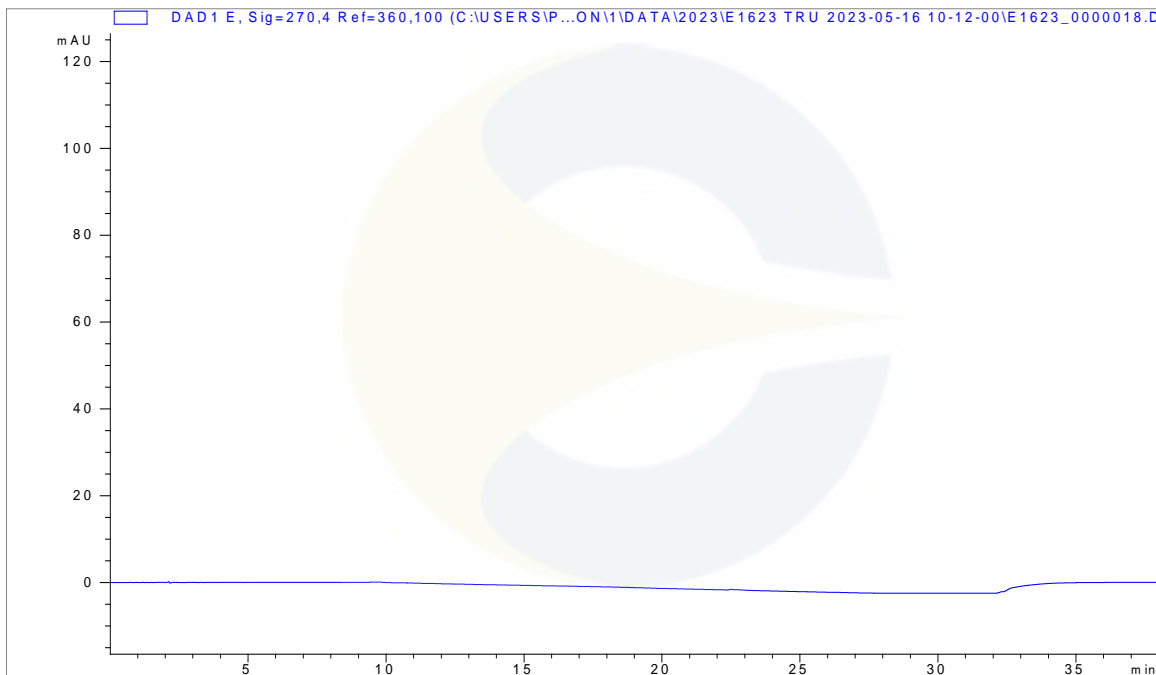
Certificate of Analysis

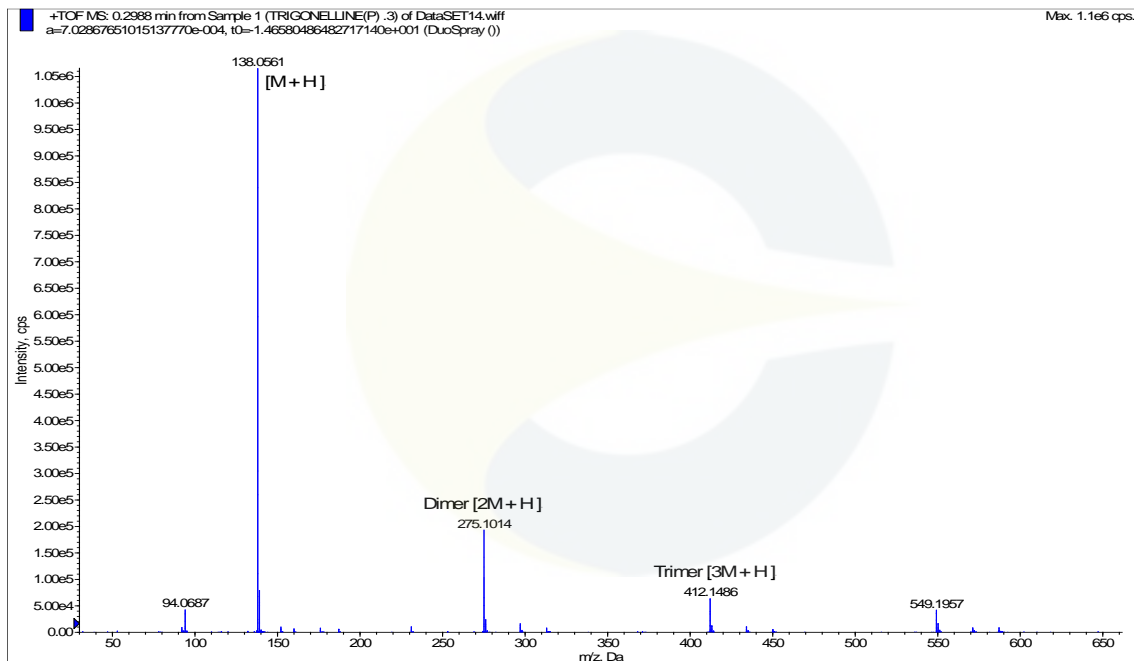
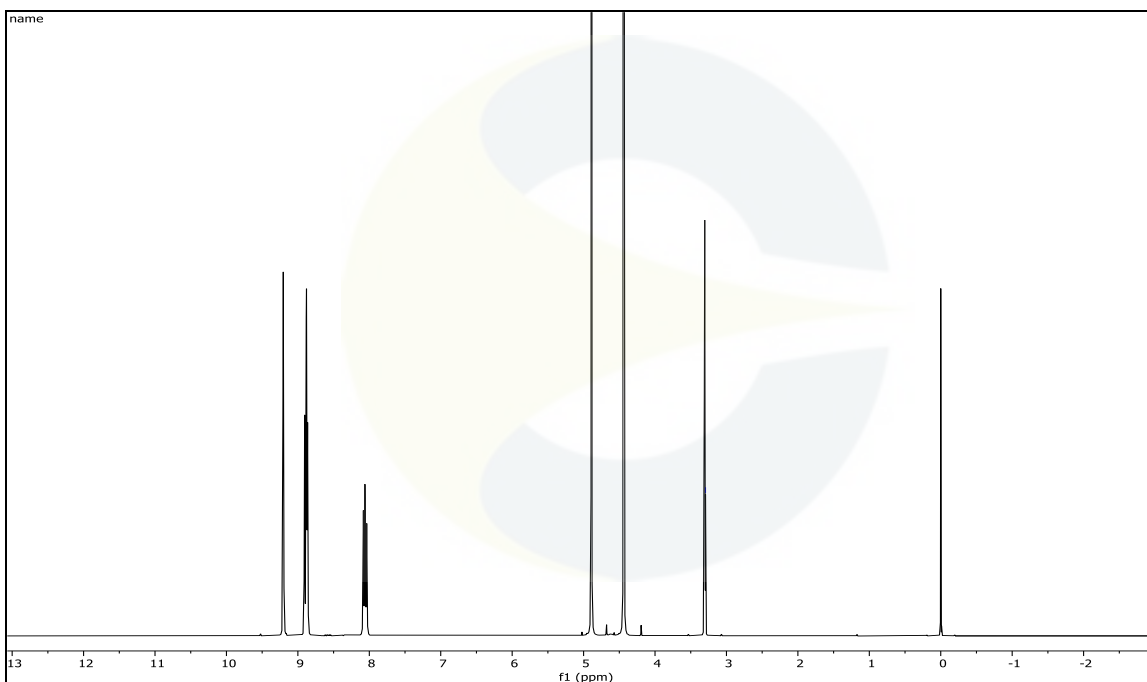
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UV SPECTRUM AT RT = 17.1 MINUTES

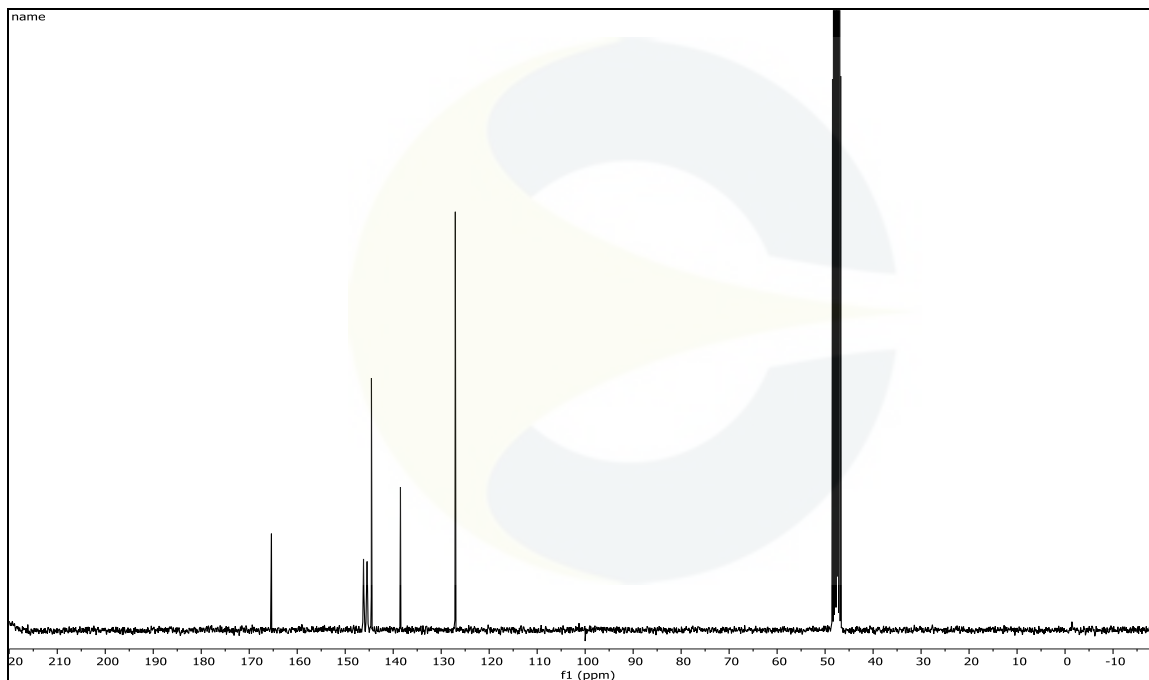


HPLC CHROMATOGRAM OF DILUENT BLANK

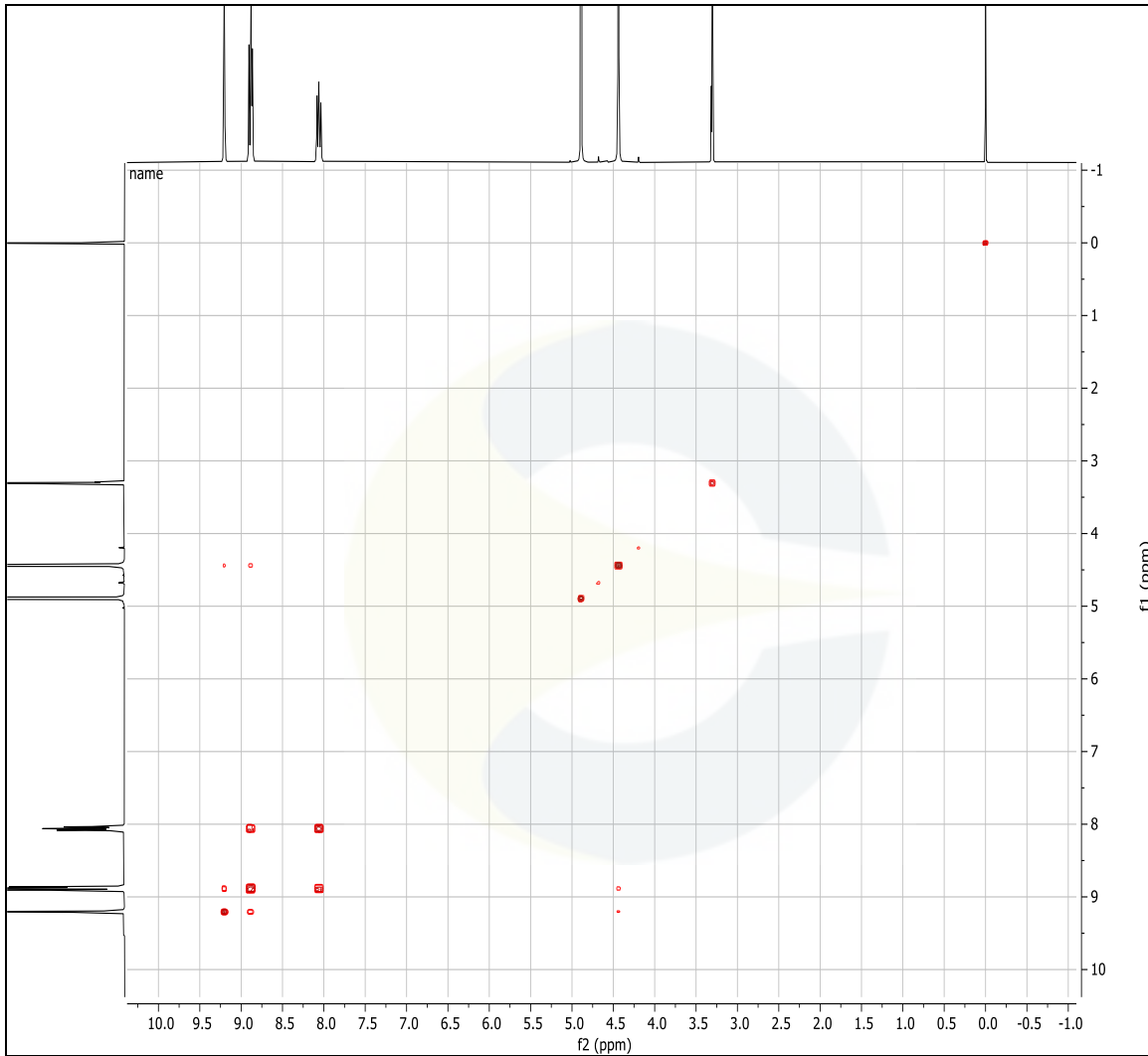


MASS SPECTRUM OF TRIGONELLINE (00020353-311)

¹H-NMR SPECTRUM OF TRIGONELLINE (00020353-311) IN CD₃OD +TMS


¹³C-NMR SPECTRUM TRIGONELLINE (00020353-311) IN CD₃OD +TMS



COSY-NMR SPECTRUM OF TRIGONELLINE (00020353-311) IN CD₃OD +TMS



REVISION HISTORY

<u>Revision History</u>	<u>Date of Revision</u>	<u>Document/Changes</u>
00	27Jun2023	New report