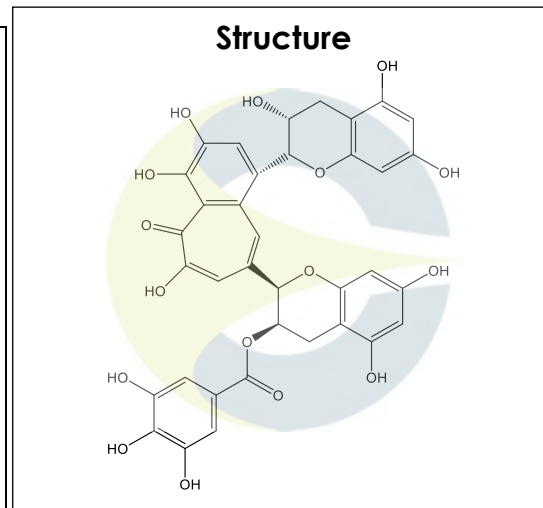


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PRODUCT NAME	Theaflavin-3-gallate
PART NUMBER	00020258
STANDARD TYPE	Primary (P)
LOT NUMBER	00020258-841
REPORT NUMBER	CDXA-RSS-7311-01
SAMPLE NUMBER	CDXP-16-012620
DATE OF SAMPLE	10/03/2016
DATE OF RE-EVALUATION	11/05/2020
DATE OF REPORT	12/08/2020



CHEMICAL NAMES	Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-2-[1-[(2R,3R)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-5H-benzocyclohepten-8-yl]-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester; Theaflavin 2A; Theaflavin 3-O-gallate; Theaflavin monogallate
CHEMICAL FORMULA	C ₃₆ H ₂₈ O ₁₆
MOLECULAR WEIGHT (MW)	716.60
CHEMICAL FAMILY	Catechins
CAS NUMBER	[30462-34-1]
EC#(EINECS)	N/A
RTECS	DH9015000

ANALYTICAL RESULTS

TEST	METHOD	SPECIFICATION	RESULT
Adjusted Purity	NA	≥ 85%	85.2%
UHPLC	0.700.10.2.METH74	≥ 90%	96.2%
NMR	4.5.3-CD-4.0-000338	Conforms to structure	Conforms to structure
Mass Spectrum	99.1-CDXA-2.0-000126	Conforms	Conforms
Residual Solvent	99.1-CD-9.0-000115	NA	Ethanol – 0.4% Hexane – 0.1% Ethyl Acetate – 0.5% Acetone – < 0.1% MTBE – < 0.1%
Water	0.700.12.37	NA	10.4%
Appearance	NA	NA	Red Powder

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ADJUSTED PURITY: 85.2% IS BASED ON (100 - 1.0 SOLVENTS - 10.4 WATER) X 96.2% HPLC

STORAGE CONDITIONS

STORAGE -20 °C in a dry place.
EXPIRATION DATE 11/2025 under the above conditions.

ANALYTICAL CONDITIONS

INSTRUMENT AGILENT 1290 HPLC UV-VIS (DAD); AGILENT 1100 ION TRAP

COLUMN Kinetex Phenyl-Hexyl 50 x 2.10 mm, 2.6 µm particle size

MOBILE PHASE A – 0.1% Phosphoric acid in (97:2:1) Milli-Q water: Acetonitrile: Methanol
B – Methanol, C – Acetonitrile
0% B and 0% C increasing to 10% B and 0% C over 2 min, then increasing to 15% B and 15% C over 4 min, then decreasing to 10% B and increasing to 20% C over 2 min, then decreasing to 5% B and increasing to 35% C over 4 min, then increasing to 10% B and 50% C over 0.5 min, then increasing to 55% C over 3 min, and decreasing to 0% b and 0% C over 0.5 min.

COLUMN TEMP. 25 °C

FLOW RATE 0.6 mL/minute

INJECTION VOL. 0.4 µL

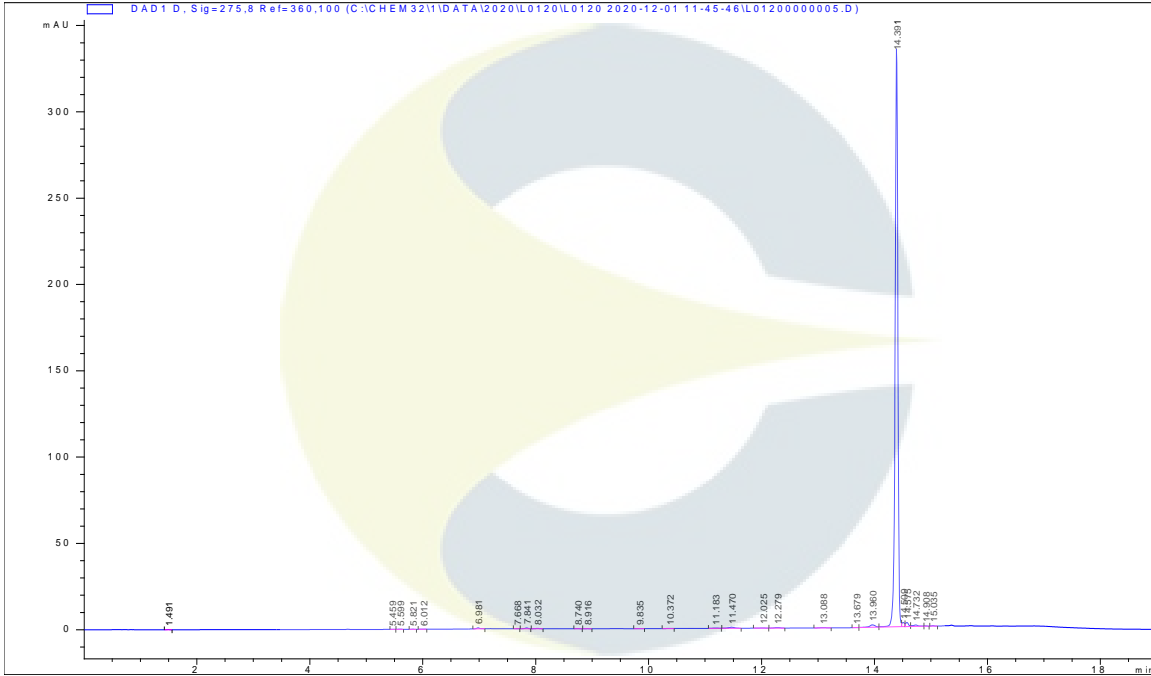
INJECTION CONC. 1.1 mg/mL in Methanol

DETECTION 275 ± 4 nm

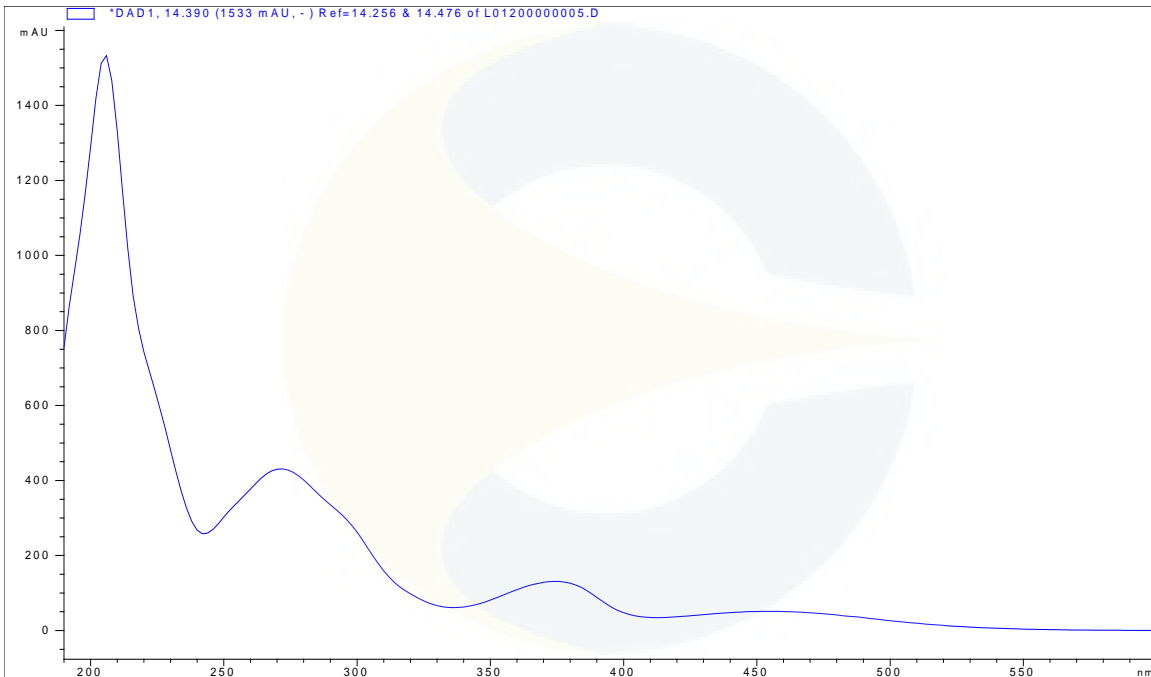
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HPLC CHROMATOGRAM OF THEAFLAVIN-3-GALLATE (CDXP-16-012620)

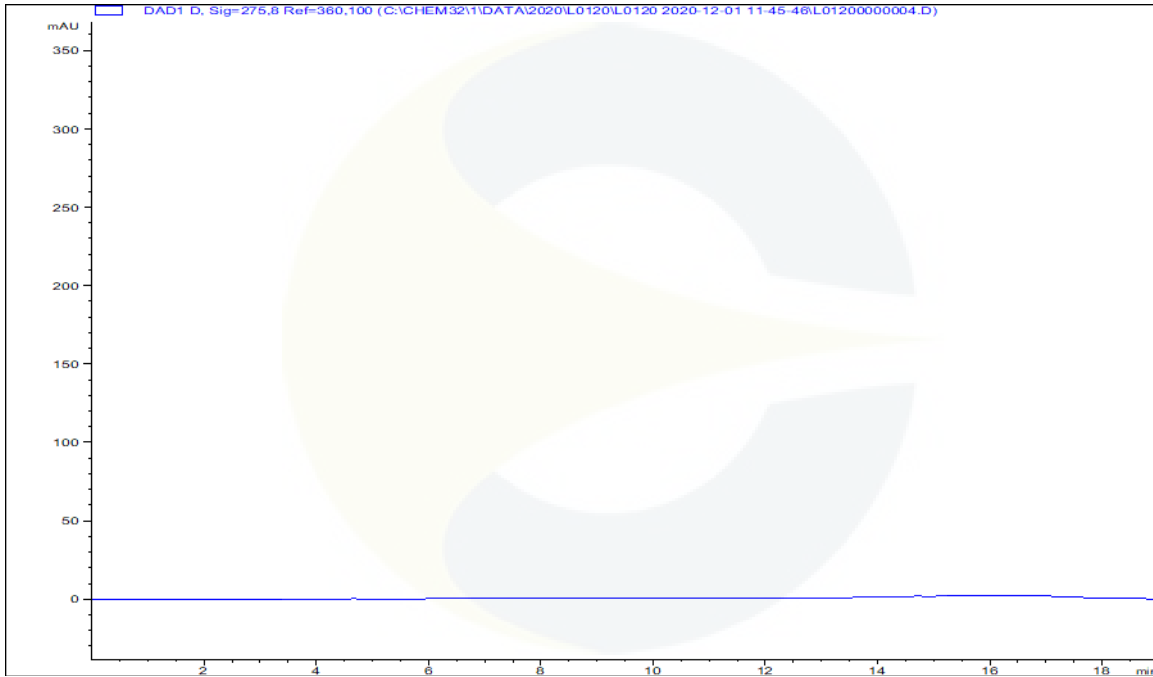


UV SPECTRUM AT 14.4 MINUTES

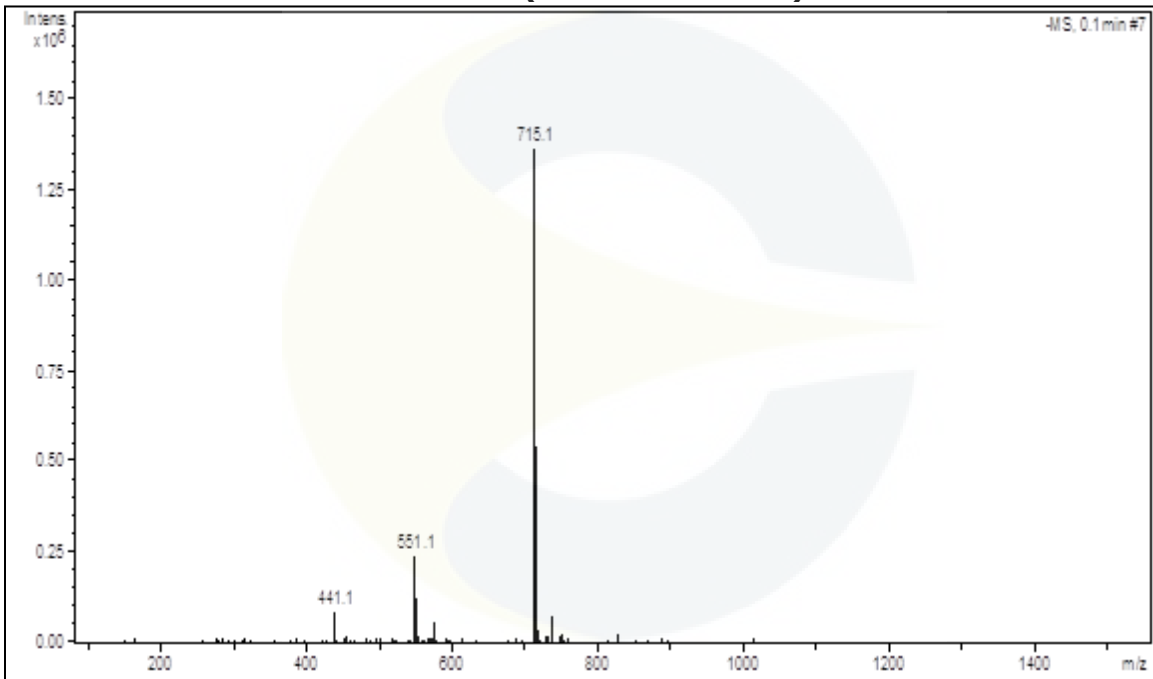


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HPLC CHROMATOGRAM OF DILUENT BLANK

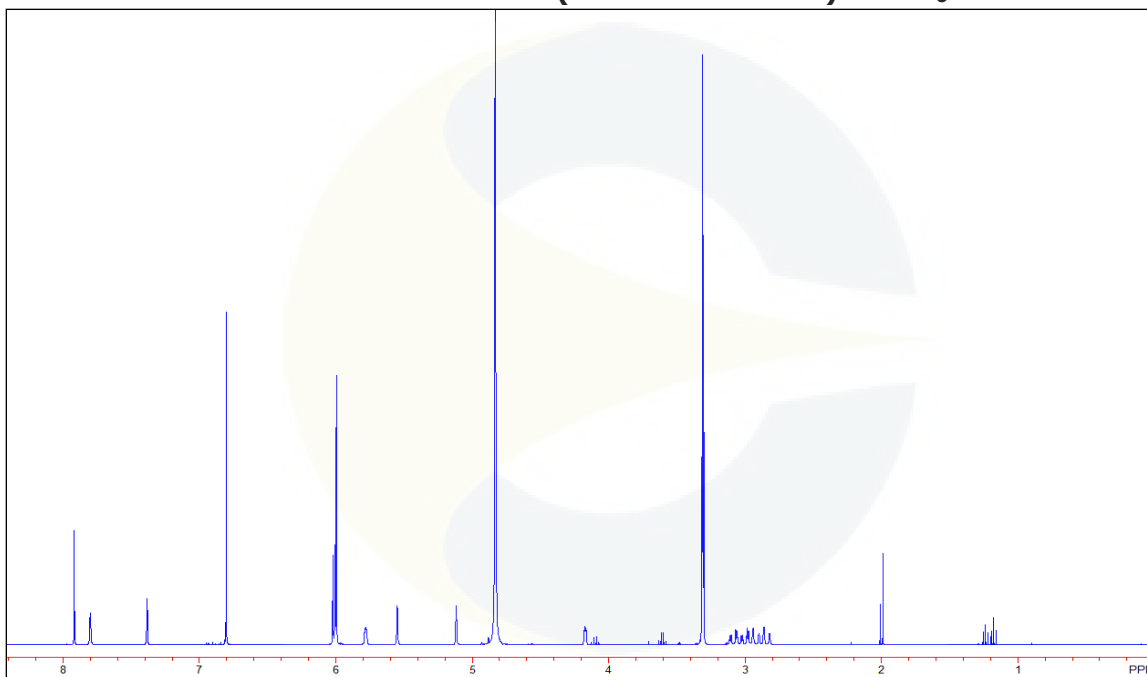


MASS SPECTRUM OF THEAFLAVIN-3-GALLATE (CDXP-16-012620)

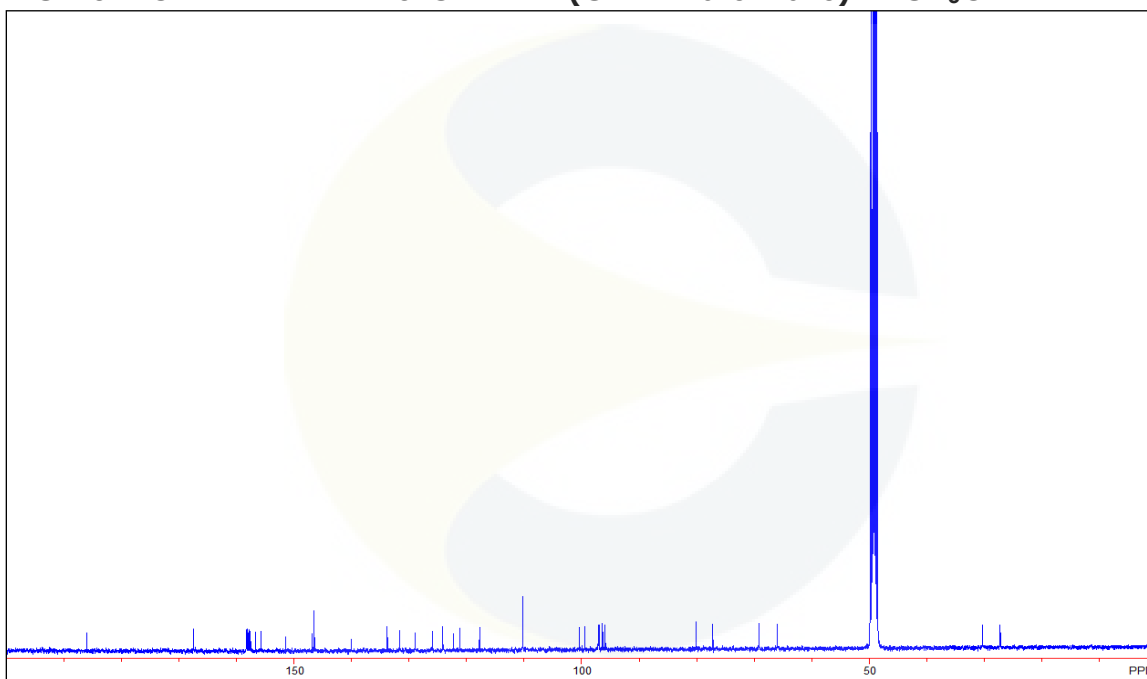


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¹H-NMR SPECTRUM OF THEAFLAVIN-3-GALLATE (CDXP-16-012620) IN CD₃OD

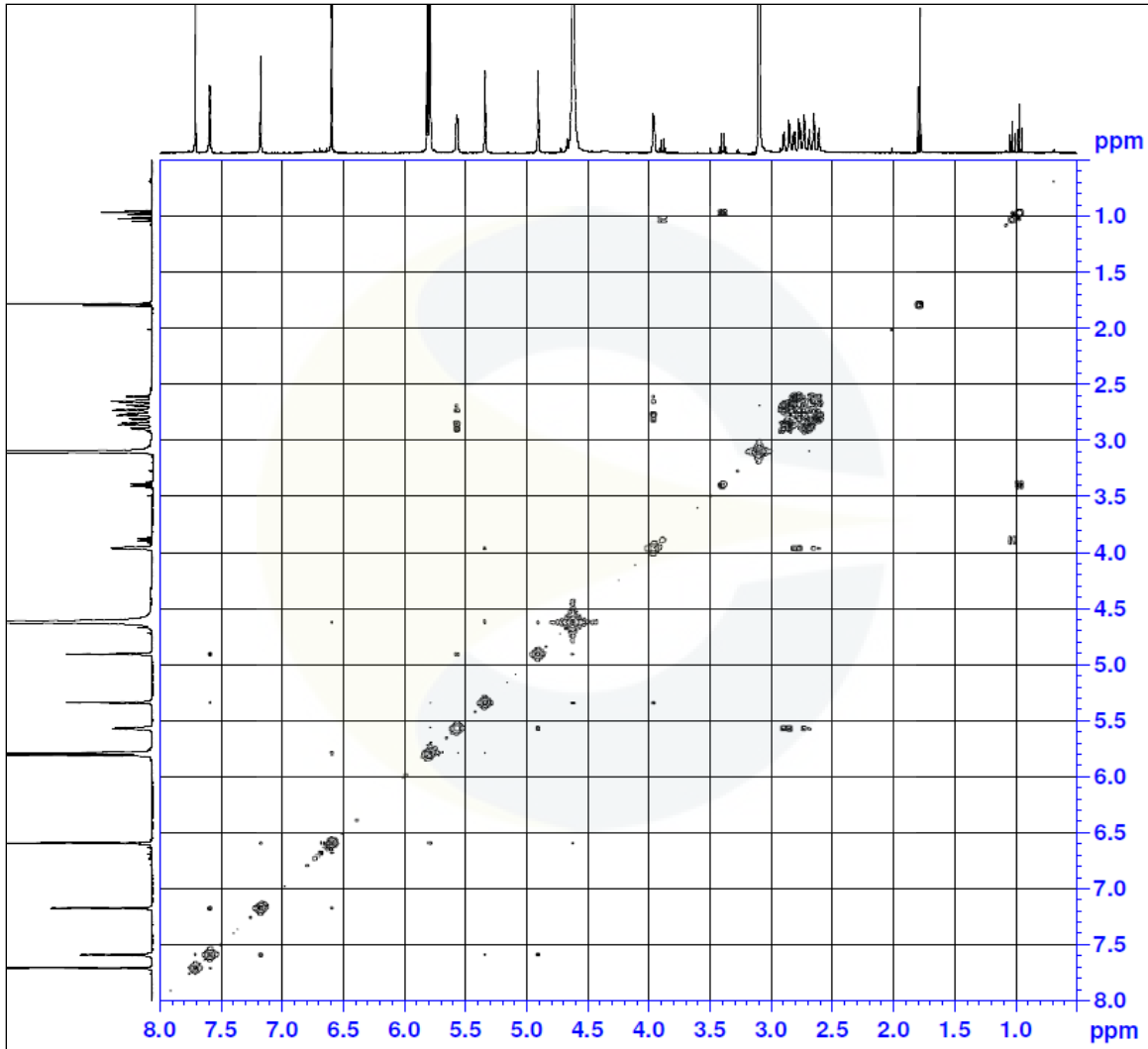


¹³C-NMR SPECTRUM OF THEAFLAVIN-3-GALLATE (CDXP-16-012620) IN CD₃OD



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COSY-NMR SPECTRUM OF THEAFLAVIN-3-GALLATE (CDXP-16-012620) IN CD₃OD



REVISION HISTORY

<u>Revision History</u>	<u>Date of Revision</u>	<u>Document/Changes</u>
00	11/09/2016	New report
01	12/08/2020	Material passed reevaluation by HPLC and KF. Removed melting point. Added RTECS number. Updated expiration date, HPLC chromatograms, HPLC and KF results, and analytical conditions.

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