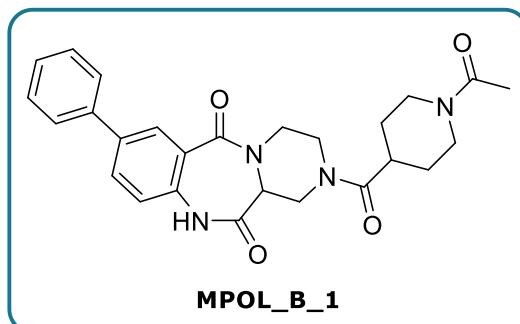




CERTIFICATE OF ANALYSIS

SHEET 1/3



COMPOUND IDENTITY

BATCH IDENTIFIER:	ITALBI_0103B
COMPOUND IDENTIFIERS:	MPOL_B_1
CHEMICAL NAME:	13-(1-acetylpiperidine-4-carbonyl)-5-phenyl-1,9,13-triazatricyclo[9.4.0.0 ^{3,8}]pentadeca-3(8),4,6-triene-2,10-dione
CAS NUMBER:	-
NOVALIX QUOTE:	NVX230227
BARCODE:	-
PROJECT IDENTIFIER:	-
PO NUMBER:	-

COMPOUND DESCRIPTORS

FREE BASE FORMULA:	C ₂₆ H ₂₈ N ₄ O ₄
FREE BASE MOLECULAR WEIGHT:	460.53 g.mol ⁻¹
SALT FORMULA:	-
SALT MOLECULAR WEIGHT:	-
PHYSICAL ASPECT:	White powder
STABILITY:	-
KNOWN SOLUBILITY:	DMSO, DCM

No toxicity data available. For R&D use only. The information provided in this document is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. This information is based on the present state of our knowledge and is applicable to the product with regard to the appropriate safety precautions.

COMPOUND ANALYTICAL SPECIFICATIONS

IDENTITY DETERMINATION METHOD(S): MS, ¹H NMR

ACCEPTANCE CRITERIA: in accordance with the expected structure

PURITY DETERMINATION METHOD(S): LCMS, with UV detection @ 220 nm

ACCEPTANCE CRITERIA: > 95.0 %

IMPURITY DETERMINATION METHOD(S): -

ACCEPTANCE CRITERIA:

COMPOUND ANALYSIS

LC/MS:

METHOD REFERENCE: AN01_001_053

COMPOUND UV AREA: 99.3 %

COLUMN: Poroshell 120 EC-C18

ELUTION GRADIENT[‡]: Water (+0.2 wt % NH₄HCO₃) / Acetonitrile: from 98:2 to 0:100

DETECTION: UV (220 nm)

MASS DETECTION: ESI+ & ESI-

EXACT MASS: 460.21

MAIN MASS PEAKS: 461.2 [M+H]⁺ / 459.1 [M-H]⁻

NOTES:

[‡]: FA: Formic acid; TFA: Trifluoroacetic acid**NMR:**¹H FREQUENCY: 500 MHzSOLVENT 1: DMSO-d₆ SOLVENT 2: -RESIDUAL SOLVENT (in wt%): 0.37 wt % of DCM and 0.32 wt % of Et₂O

OTHER IMPURITIES: Presence of minor aliphatic impurities

NOTES: *in accordance with expected structure. Presence of rotamers*¹³C FREQUENCY: N/A

SOLVENT: -

NOTES: N/A.

¹H QUANTITATIVE NMR[#]: -[#]: as described in *Anal. Chem.* **2014**, 86, 11474-11480 & references herein

No toxicity data available. For R&D use only. The information provided in this document is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. This information is based on the present state of our knowledge and is applicable to the product with regard to the appropriate safety precautions.

RESULT

- ☒ This sample is compliant with requested specifications
- ☐ Within the limits of the analyses performed to date, this sample is compliant with requested specifications. Remaining analyses will be performed at client facilities
Comments:
- ☐ This sample is not compliant with requested specifications
Comments: -

NOTES

CONTACT: Dr. Hajer Abdelkafi
CHEMIST: Dr. Imen Talbi

ANALYSIS DATE: 14th November 2023
AMOUNT DELIVERED: 9.00 mg

RETEST DATE: -

REVIEWED BY: Dr. Hajer Abdelkafi

REVIEW DATE: 17th November 2023



No toxicity data available. For R&D use only. The information provided in this document is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. This information is based on the present state of our knowledge and is applicable to the product with regard to the appropriate safety precautions.

LCMS ITALBI_0103B

Data file: C:\Users\Public\Documents\ChemStation\1\Data\2023\14-11-23\ITALBI_0103B_7037.D

Injection date: 11/14/2023 9:24:07 PM

Location: P2-C-05

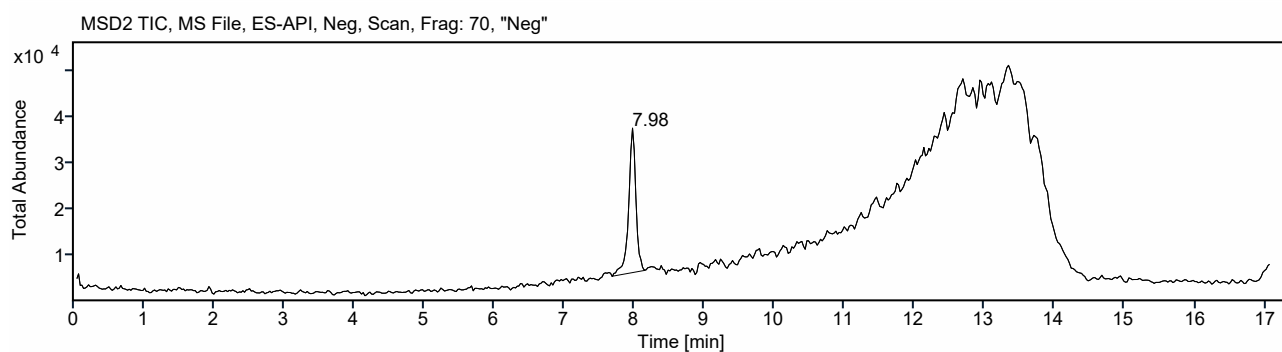
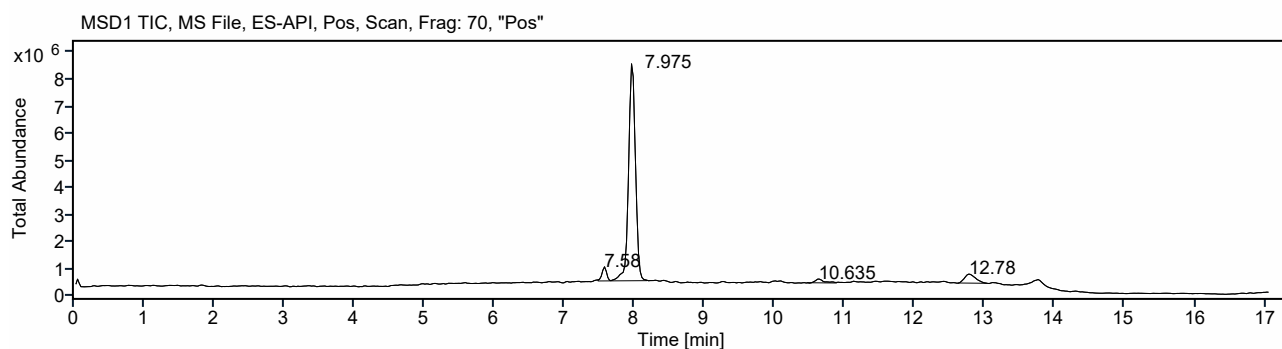
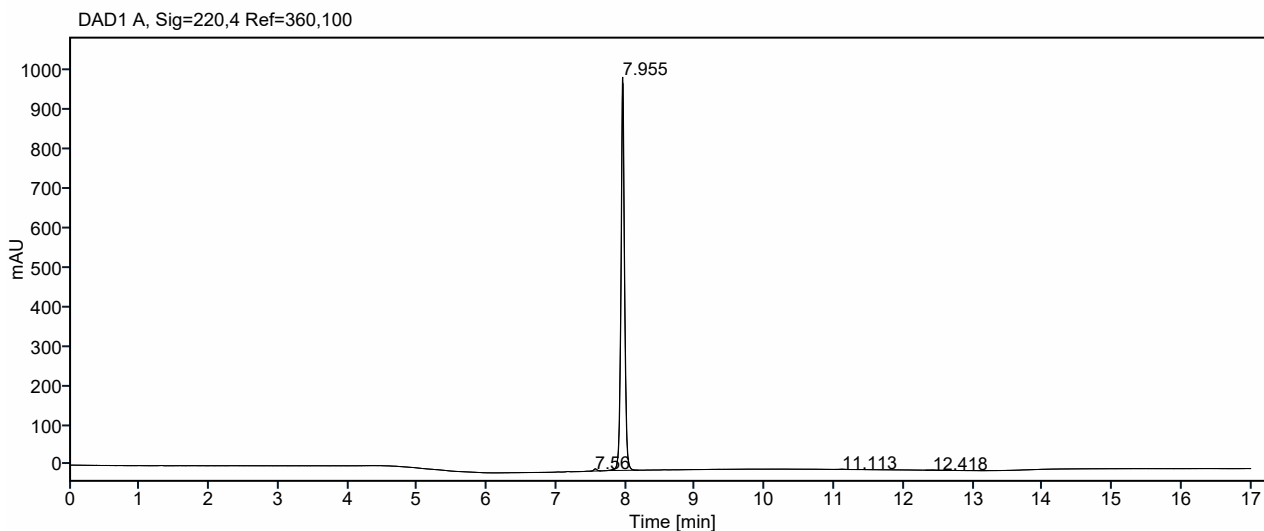
Acq. method: AN01_001_053_pos_neg.M

Inj. vol (μL) 0.500

Analysis method: AN01_001_053_pos_neg.M

Processing Method: Process UV, Process MS

Column name: Poroshell 120 EC-C18



LCMS ITALBI_0103B

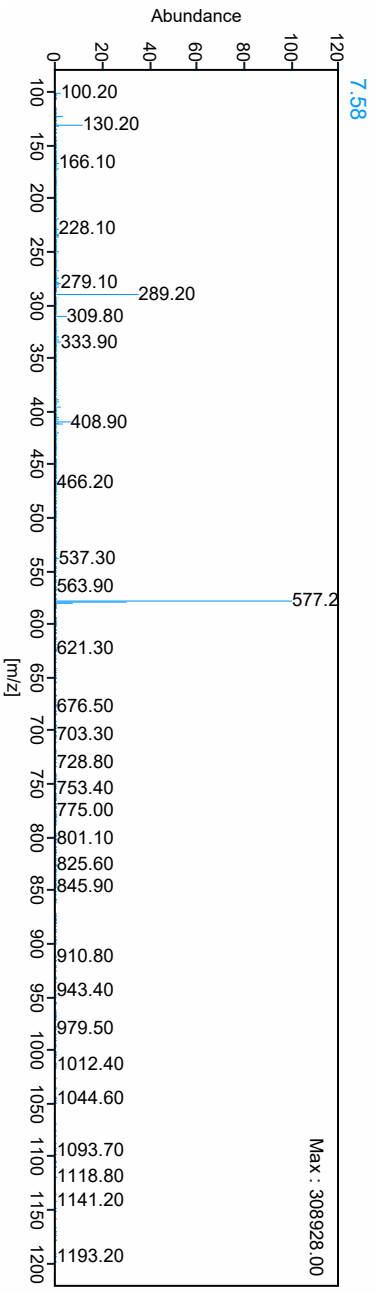
Signal: DAD1 A, Sig=220,4 Ref=360,100

	<i>Rt min</i>	<i>Area</i>	<i>Height</i>	<i>Area%</i>
	7.56	18	6	0.5
	7.95	3537	1002	99.3
	11.11	5	1	0.1
	12.42	3	1	0.1
	Sum	3563		100.0

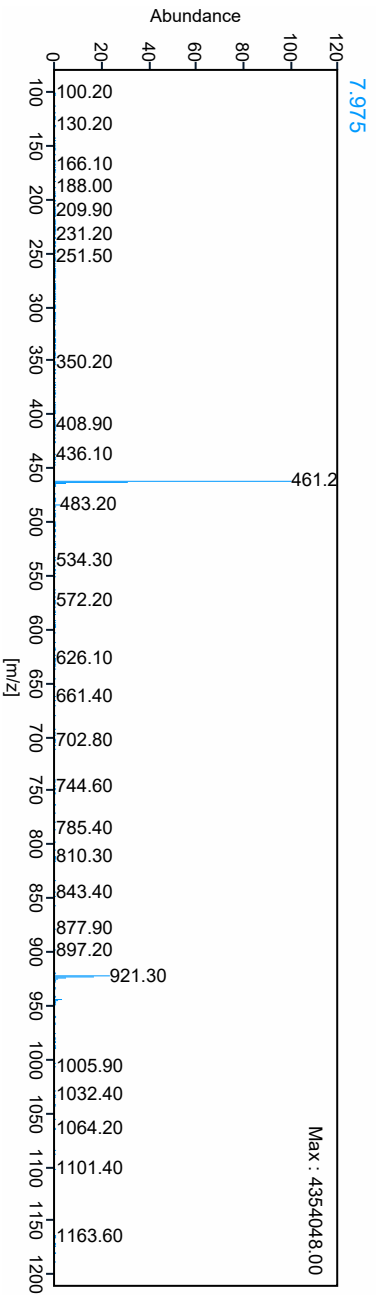
LCMS ITALBI_0103B

Signal MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70, "Pos"

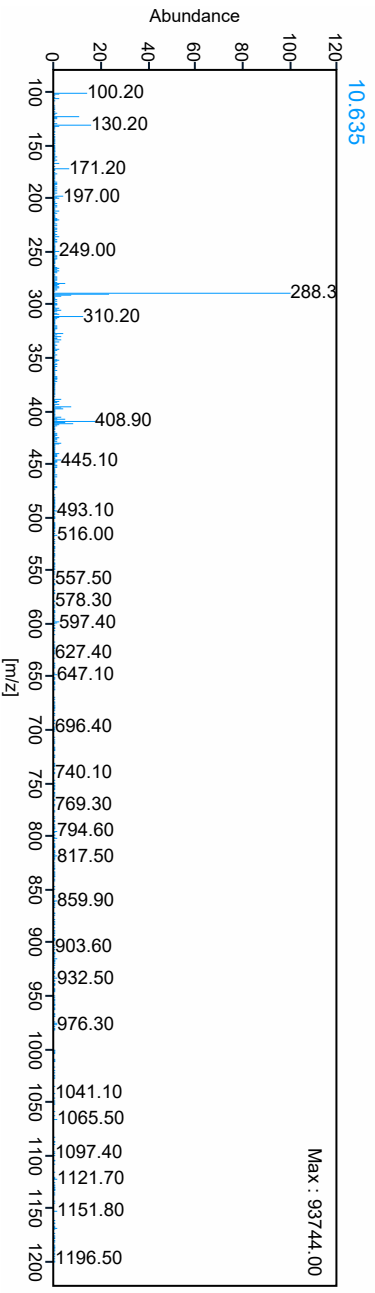
Peak RT 7.580



Peak RT 7.975

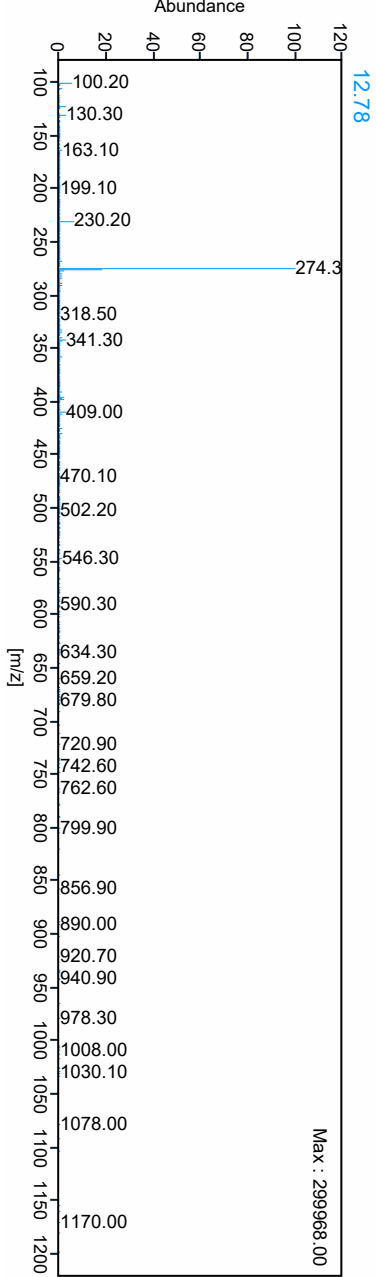


Peak RT 10.635



LCMS ITALBI_0103B

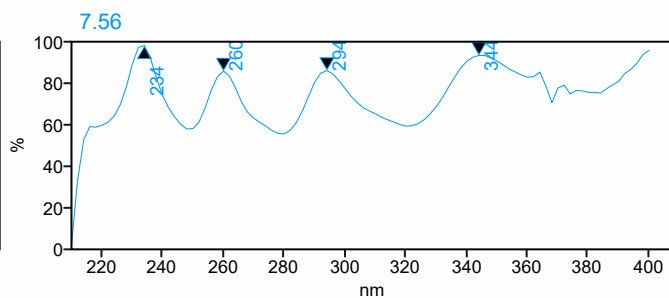
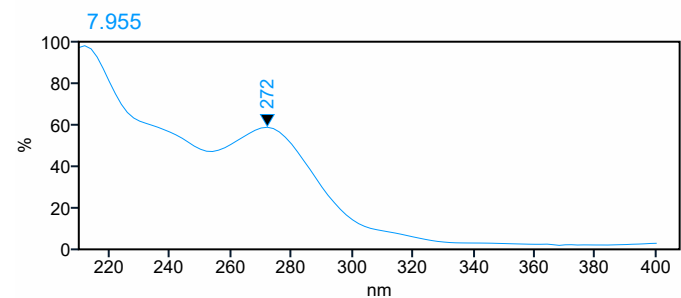
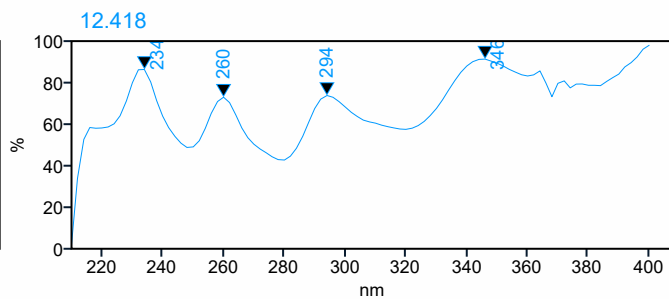
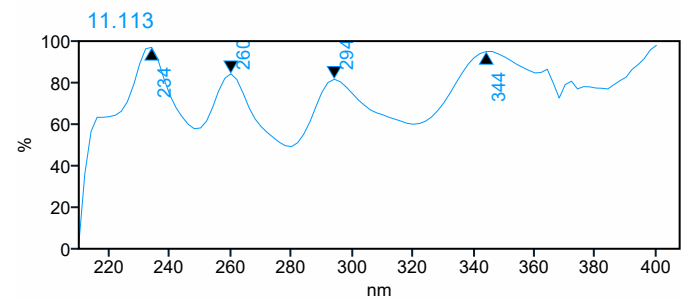
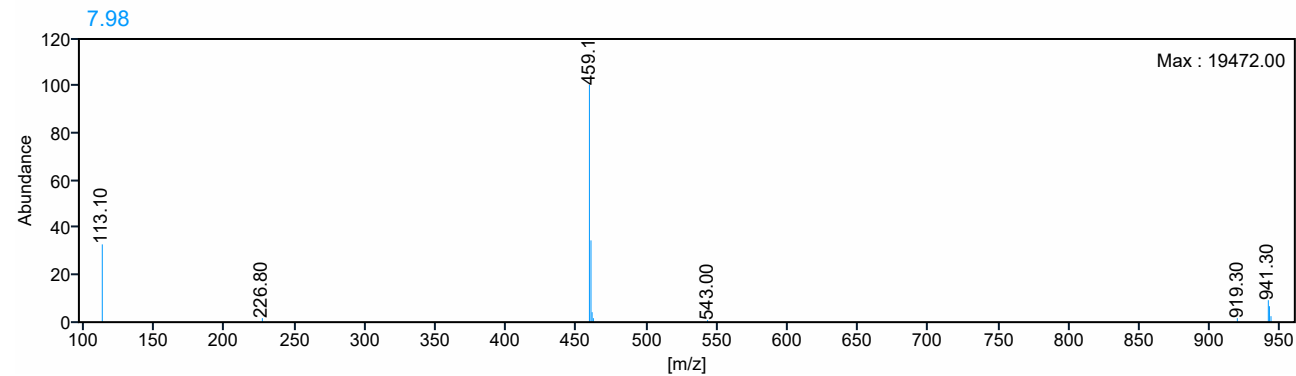
Peak RT 12.780



LCMS ITALBI_0103B

Signal MSD2 TIC, MS File, ES-API, Neg, Scan, Frag: 70, "Neg"

Peak RT 7.980



ITALBI_0103B 1 (1D 1H) DMSO 500MHz

