Supplementary Information (SI) for RSC Medicinal Chemistry. This journal is © The Royal Society of Chemistry 2025



CERTIFICATE OF ANALYSIS

SHEET 1/3

COMPOUND IDENTITY

BATCH IDENTIFIER: NNAHDI_0119A
COMPOUND IDENTIFIERS: MPOL D 1

(6S)-6-[3-(2H-1,3-benzodioxol-5-yl)-1,2,4-

oxadiazol-5-yl]-N-(4-methylphenyl)-

CHEMICAL NAME: 3H,4H,5H,6H,7H-imidazo[4,5-c]pyridine-5-

carboxamide

CAS NUMBER: -

NOVALIX QUOTE: NVX230227

BARCODE: PROJECT IDENTIFIER: PO NUMBER: -

COMPOUND DESCRIPTORS

FREE BASE FORMULA: $C_{23}H_{20}N_6O_4$ FREE BASE MOLECULAR WEIGHT: $444.45 \text{ g.mol}^{-1}$

SALT FORMULA: SALT MOLECULAR WEIGHT: -

PHYSICAL ASPECT: White powder

STABILITY: -

KNOWN SOLUBILITY: DMSO, DCM, CDCl3

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.



CERTIFICATE OF ANALYSIS

SHEET 2/3

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): nature and content of impurities

ACCEPTANCE CRITERIA:

COMPOUND ANALYSIS

LC/MS:

METHOD REFERENCE: AN01_001_053

COMPOUND UV AREA: 97.7 % 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: 444.15

MAIN MASS PEAKS: 445.1 [M+H]+ / 443.1 [M-H]-

Notes:

NMR:

¹H Frequency: 500 MHz Solvent 1: DMSO-d6 Solvent 2: -

RESIDUAL SOLVENT (in wt%):

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[#]: -

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^{‡:} FA: Formic acid; TFA: Trifluoroacetic acid

^{#:} as described in *Anal. Chem.* **2014**, 86, 11474-11480 & references herein



CERTIFICATE OF ANALYSIS

SHEET 3/3

RESULT

☐ 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 ANALYSIS DATE: 22th September 2023

CHEMIST: Nadia Nahdi AMOUNT DELIVERED: 8.00 mg

RETEST DATE: -

REVIEWED BY: Dr. Hajer Abdelkafi REVIEW DATE: 14th November 2023



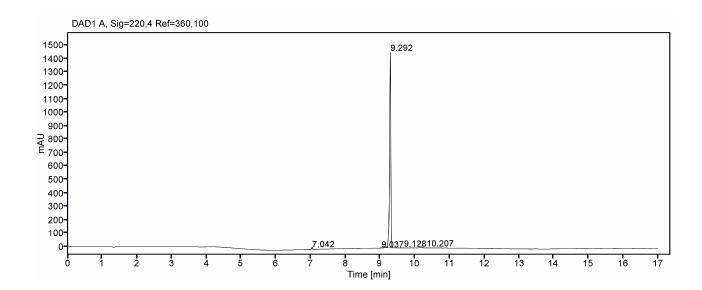
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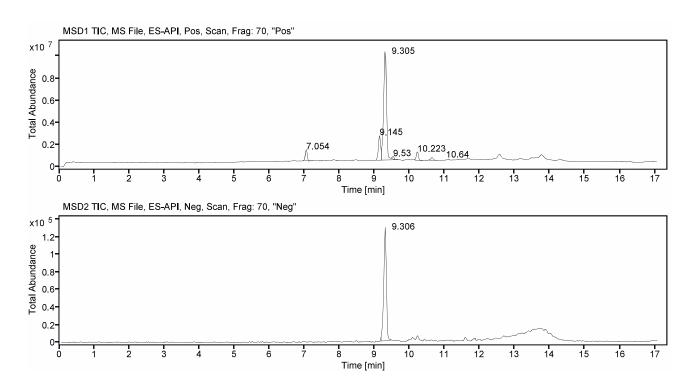
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 P1-F-05

 Acq. method:
 AN01_001_053_pos_neg.M
 Inj. vol (μL)
 1.000

Analysis method: AN01_001_053_pos_neg.M Processing Method: Process UV, Process MS

Column name: Poroshell 120 EC-C18



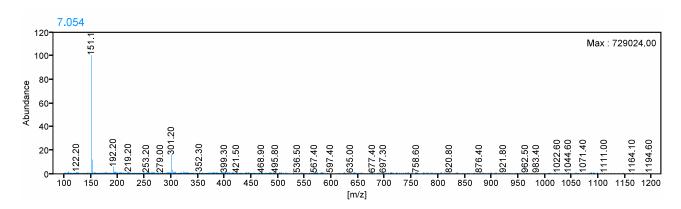


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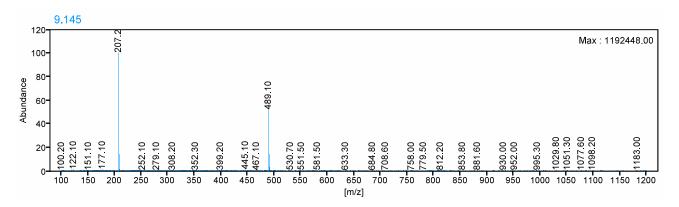
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9.13	18	8	0.5
9.29	3665	1468	97.7
10.21	24	10	0.6
Sum	3753		100.0

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

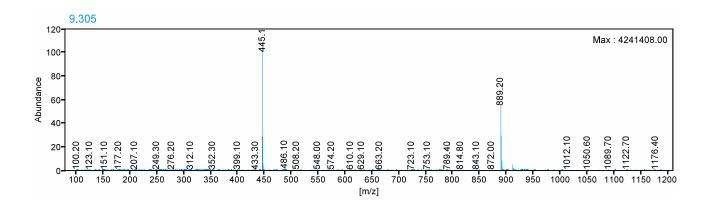
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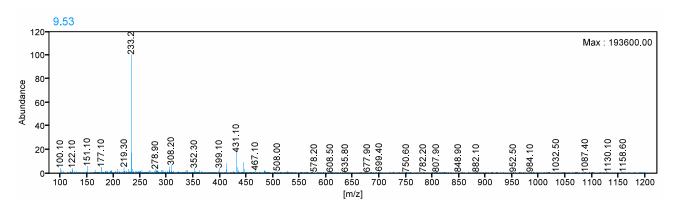
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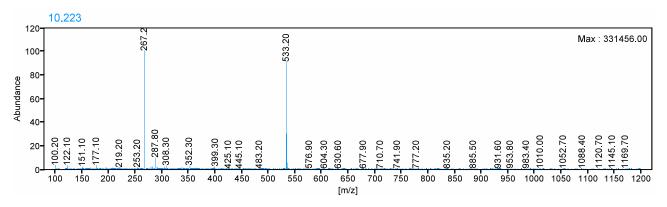
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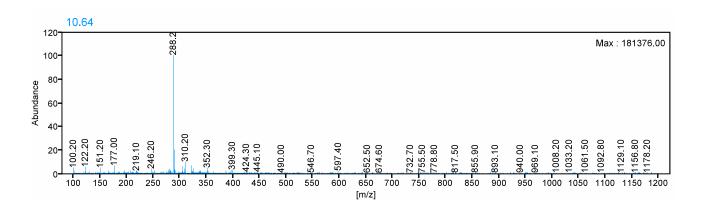
Peak RT 9.530



Peak RT 10.223



Peak RT 10.640



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

Peak RT 9.306

