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NATIONAL FORENSIC LABORATORY
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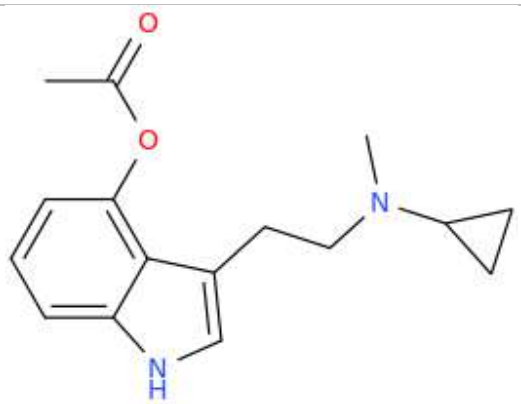
ANALYTICAL REPORT

4-AcO-McPT (C16H20N2O2)

3-{2-[cyclopropyl(methyl)amino]ethyl}-1H-indol-4-yl acetate

Remark – other NPS detected: none

Sample ID:	2028-18
Sample description:	powder
Sample type:	test purchase /NFL- purchasing
Date of entry (DD/MM/YYYY) into NFL database:	25/10/2023
Report updates (if any) will be published here:	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance identified - structure[1] (base form)	
Systematic name	3-{2-[cyclopropyl(methyl)amino]ethyl}-1H-indol-4-yl acetate
Other names	
Formula (per base form)	C16H20N2O2
M_w (g/mol)	272,35
Salt form/anions detected	fumarate
StdInChIKey (per base form)	LTVOZYTYGWHKES-UHFFFAOYSA-N
Other NPS detected	none
Additional info (purity..)	minor impurities observed by GC-MS

[1] Created by OPSIN free tool: http://opsin.ch.cam.ac.uk/ **DOI:** 10.1021/ci100384d

Report updates

date	comments (explanation)

Instrumental methods (if applied) in NFL

1. GC-MS (Agilent): GC-method is RT locked to tetracosane (9.258 min). Injection volume 1 µl and split mode (1:50). Injector temperature: 280 0C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 190 ^{0}C at rate 8 ^{0}C/min, then heating up to 293 0C at a rate of 18 ^{0}C/min, hold for 6.1 min, then heating at 50 ^{0}C/min up to 325 ^{0}C and finally 9.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300 until 6 min) amu.

2. HPLC-TOF (Agilent): 6230B TOF with Agilent 1260 Infinity HPLC with binary pump, column: Zorbax Eclipse XDB-C18, 50 x 4.6 mm, 1.8 micron. Mobile phases (A) 0.1% formic acid and 1mM ammonium formate in water; (B) 0.1% formic acid in methanol (B). Gradient: starting at 5% B, changing to 40% B over 4 min, then to 70% over 2 min and in 5 min to 100%, hold 1 min and back to 5%, equilibration for 1.7 min. The flow rate: 1.0 ml/min; Injection volume 1 µl. MS parameters: 2GHz, Extended Dynamic range mode to a maximum of 1700 amu, acquisition rate 1.30 spectra/sec. Sample ionisation: by Agilent Jet Stream technology (Dual AJS ESI). Ion source: positive ion scan mode with mass scanning from 82 to 1000 amu. Other TOF parameters: drying gas (N2) and sheath temperature 325 °C; drying gas flow rate 6 l/min; sheath gas flow rate 8 l/min; nebulizer 25 psig; Vcap. 4000 V; nozzle 2000 V; skimmer 65 V; fragmentor 175 V and Octopole RF 750 V.

3.FTIR-ATR (Perkin Elmer): scan range 4000-400 cm-1; resolution 4cm-1

4. GC- (MS)-IR solid phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)
GC-method: Injection volume 1 µl and split mode (1:5). Injector temperature 280 ^{0}C. Chromatographic separation as above **(1).**
Split MS : IR = 1: 9.
MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.
IR (condesed (solid) phase): IR scan range 4000 to 650, resolution 4 cm^{-1} .

5. **IC** (anions) (Thermo Scientific, Dionex ICS 2100), Column: IonPac AS19, 2 x 250mm; Eluent: 10mM KOH from 0 to 10 min, 10-58 mM from 10 to 40min; Flow rate: 0.25 ml/min; Temperature: 30˚C; Suppressor: AERS 500 2mm, suppressor current 13mA; Inj. Volume: 25 µl

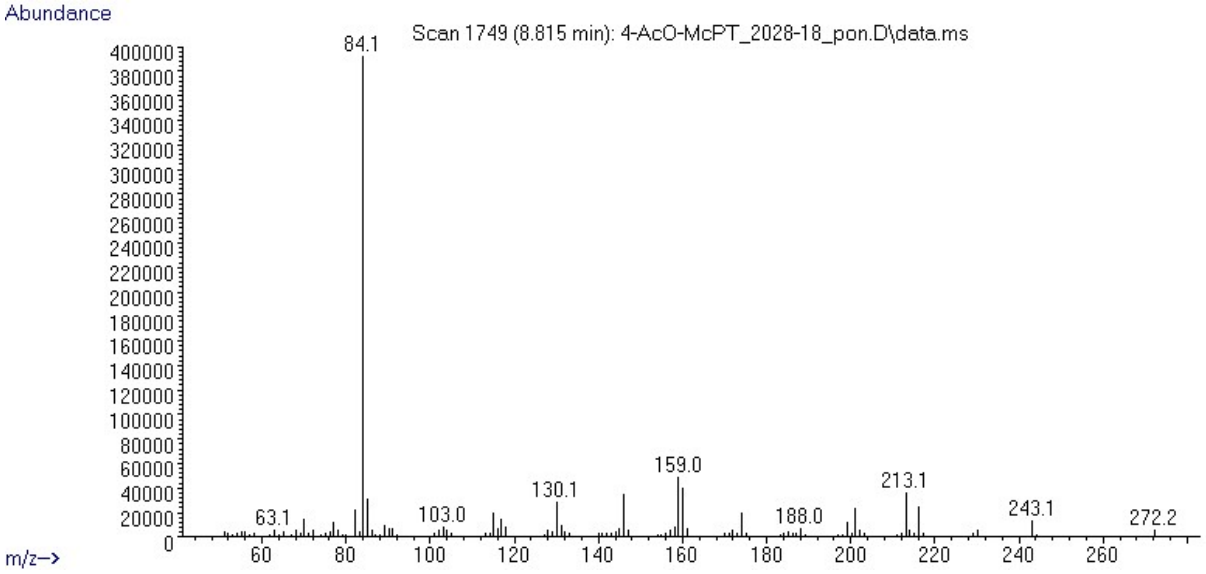
Supporting information

Solubility in	result/remark
CH_2Cl_2	partially
MeOH	soluble
H_2O	partially

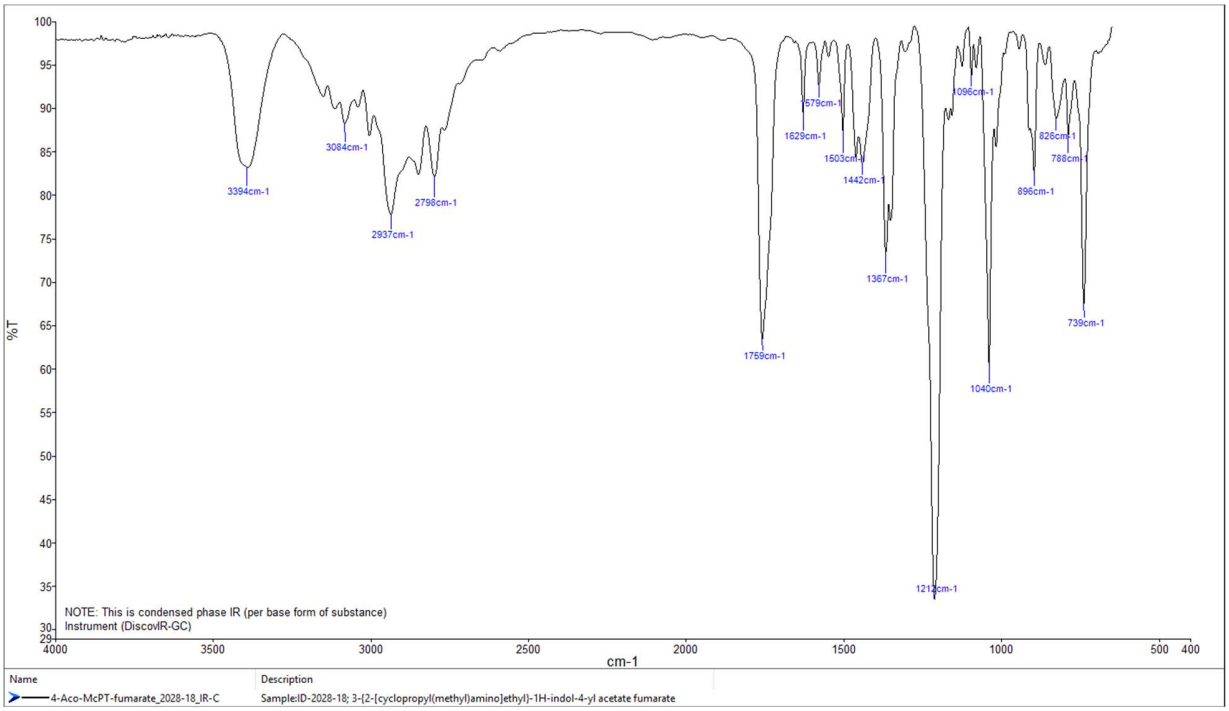
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 8,82 BP(1): 84; BP(2): 159,BP(3) :160,
HPLC-TOF	+	Exact mass (theoretical): 272,1525; measured value Δppm:-1,04; formula:C16H20N2O2
FTIR-ATR	-	direct measurement (sample as received)
FTIR (solid phase) always as base form	+	
IC (anions)	+	
NMR (in FKKT)	+	
validation		
other		

ANALYTICAL RESULTS

MS (EI)



IR (solid phase – after chromatographic separation)



TOF REPORT

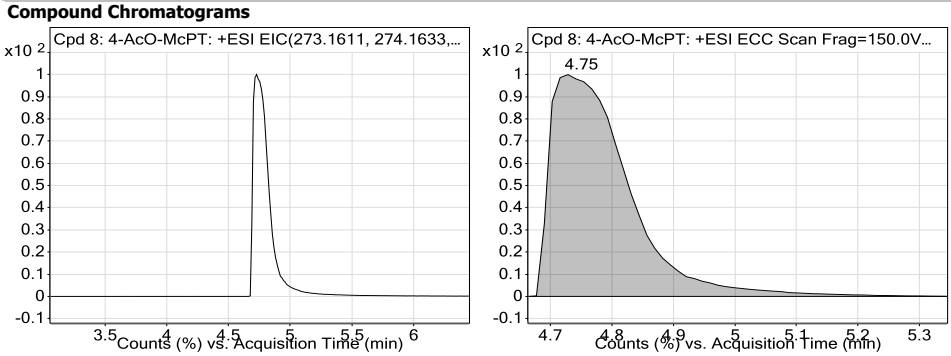
Data File	4-AcO-McPT_2028-18.d	**Sample Name**	ID 2028-18
Sample Type	Sample	**Position**	P2-F8
Instrument Name	6230B TOF LC-MS	**User Name**	TG
Acq Method	general-19_10_2018-XDB-C18-ESI+.m	**Acquired Time**	11/20/2018 11:49:52 AM
IRM Calibration Status	Success	**DA Method**	0-NPS in sorodne snovi.m
Comment	MeOH		

Compound Table

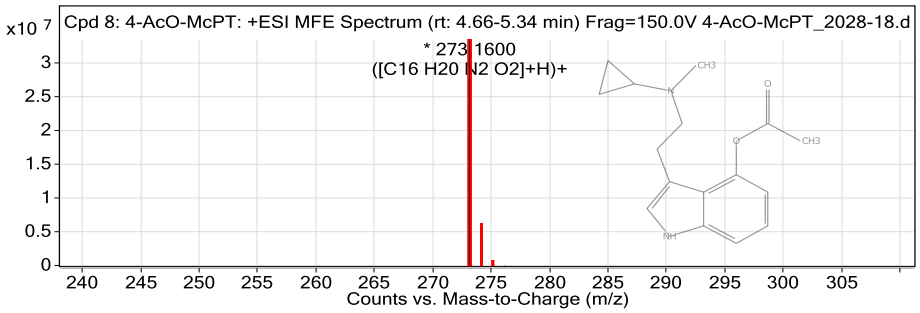
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 8: 4-AcO-McPT	4-AcO-McPT	C16 H20 N2 O2	4.75	272.1528

Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
4-AcO-McPT	273.16	4.75	272.1528	4.75	C16 H20 N2 O2	272.1525	-1.04

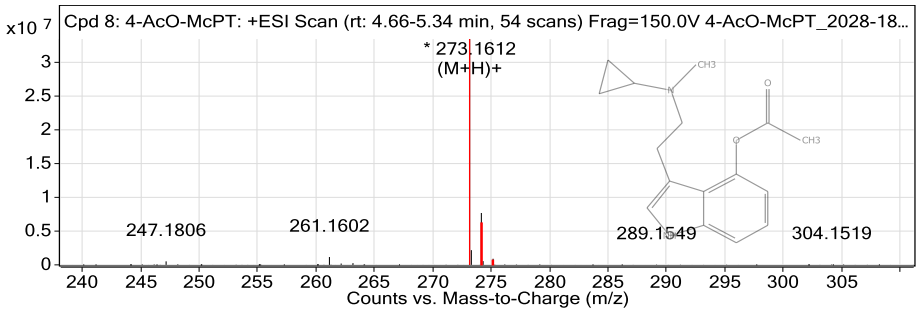
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

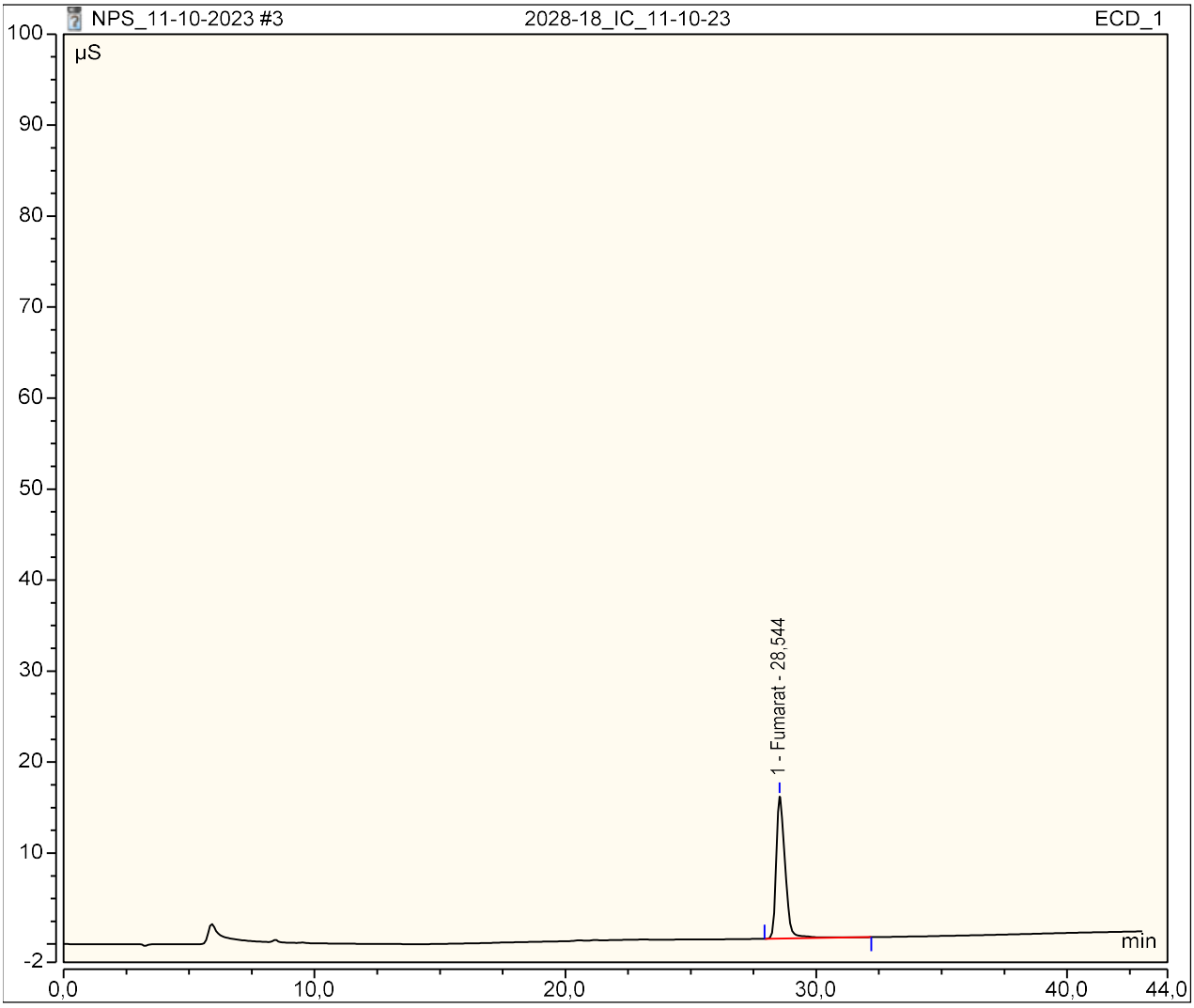
Obs. m/z	Charge	Abund	Formula	Ion/Isotope
273.16	1	33422356	C16 H20 N2 O2	(M+H)+
274.1634	1	6157142.85	C16 H20 N2 O2	(M+H)+
275.1665	1	560393.74	C16 H20 N2 O2	(M+H)+
276.1691	1	49509.51	C16 H20 N2 O2	(M+H)+

--- End Of Report ---

Peak Integration Report

Sample Name:	**2028-18_IC_11-10-23**	*Inj. Vol.:*	**25,00**
Injection Type:	**Unknown**	*Dilution Factor:*	**1,0000**
Instrument Method:	**ANIONI**	*Operator:*	**Admin**
Inj. Date / Time:	**11-Oct-2023 / 15:22**	*Run Time:*	**43,00**

No.	Time min	Peak Name	Peak Type	Area µS*min	Height µS	Amount mg/L
1	28,54	**Fumarat**	BMB	6,416	15,612	n.a.
		TOTAL:		6,42	15,61	0,00



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University
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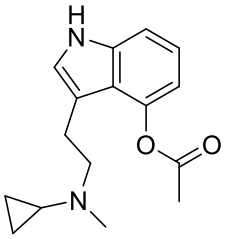
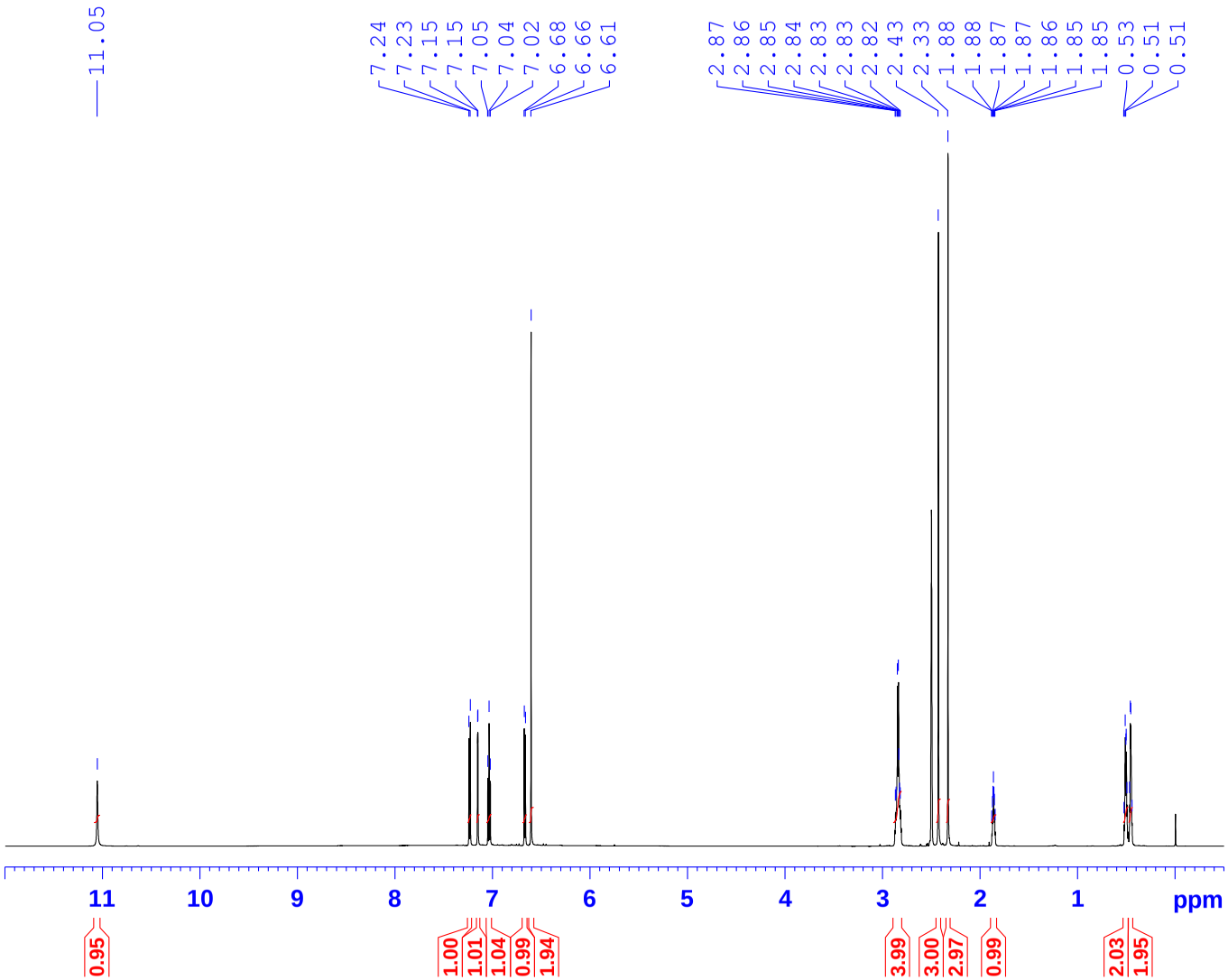
Faculty *of Chemistry*
and Chemical Technology

R E P O R T

Contract No.	C1714-21-460153 (Republic of Slovenia, Ministry of the Interior, POLICE)
Sample ID:	**2028-18**
Received date:	July 17, 2023
Our notebook code:	NFL-2028-18
NMR sample preparation:	19.6 mg dissolved in 0.6 mL DMSO-d_6
NMR experiments:	^{1}H, ^{13}C, ^{1}H–^{1}H *gs*-COSY, ^{1}H–^{13}C *gs*-HSQC, ^{1}H–^{13}C *gs*-HMBC, ^{1}H–^{15}N *gs*-HMBC
Proposed structure with formula, exact mass, molecular weight:	 Chemical Formula: $C_{16}H_{20}N_2O_2$ Exact Mass: 272,1525 Molecular Weight: 272,3480
Chemical name:	3-(2-(Cyclopropyl(methyl)amino)ethyl)-1*H*-indol-4-yl acetate
Comments:	- Structure elucidation based on 1D and 2D NMR spectra and HRMS. - The sample consists of the above compound and fumaric acid in a relative ratio of 1:1. - Sample is pure based on ^{1}H NMR spectrum.
Supporting information:	Copies of ^{1}H and ^{13}C NMR spectra, ^{1}H and ^{13}C FIDs.
Principal investigator:	Prof. Dr. Janez Košmrlj
Date of report:	July 19, 2023

NFL-2028-18
1H



Current Data Parameters

NAME	NFL-2028-18
EXPNO	10
PROCNO	1

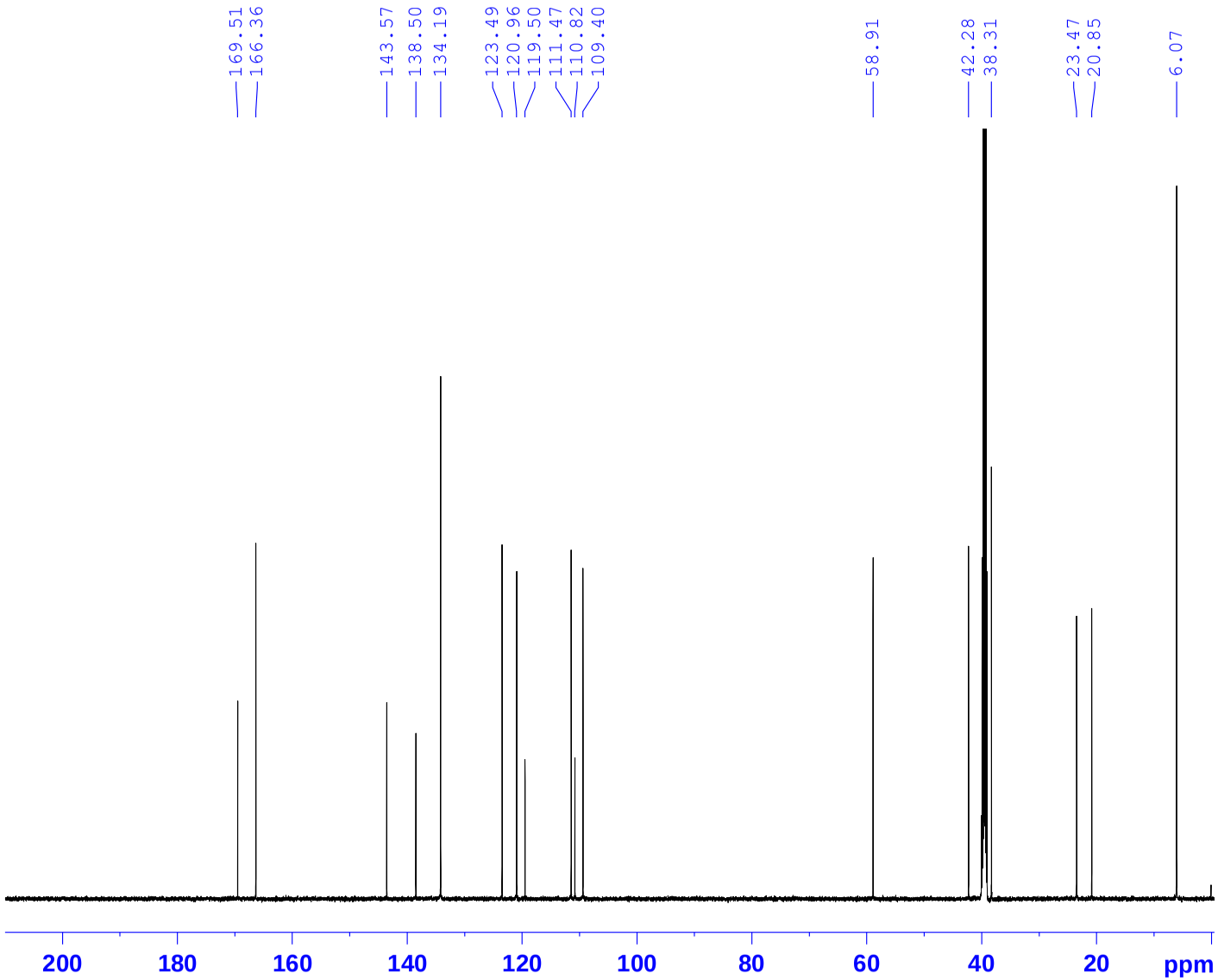
F2 - Acquisition Parameters

Date_	20230714
Time	18.31 h
INSTRUM	AV600 NEO
PROBHD	Z176567_0002 (
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	32
DS	2
SWH	11904.762 Hz
FIDRES	0.363304 Hz
AQ	2.7525120 sec
RG	63.0303
DW	42.000 usec
DE	8.79 usec
TE	298.4 K
D1	1.00000000 sec
TD0	1
SFO1	600.1337058 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
PLW1	16.51399994 W

F2 - Processing parameters

SI	65536
SF	600.1300034 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

NFL-2028-18
13C



Current Data Parameters

NAME	NFL-2028-18
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20230714	
Time	20.44	h
INSTRUM	AV600 NEO	
PROBHD	Z176567_0002 (	
PULPROG	zgpg30	
TD	65536	
SOLVENT	DMSO	
NS	4000	
DS	4	
SWH	35714.285	Hz
FIDRES	1.089913	Hz
AQ	0.9175040	sec
RG	101	
DW	14.000	usec
DE	6.50	usec
TE	300.0	K
D1	1.00000000	sec
D11	0.03000000	sec
TD0	1	
SFO1	150.9178988	MHz
NUC1	13C	
P0	4.00	usec
P1	12.00	usec
PLW1	101.26000214	W
SFO2	600.1324005	MHz
NUC2	1H	
CPDPRG[2	waltz65	
PCPD2	70.00	usec
PLW2	16.51399994	W
PLW12	0.33702001	W
PLW13	0.16952001	W

F2 - Processing parameters

SI	32768	
SF	150.9028816	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	