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NATIONAL FORENSIC LABORATORY
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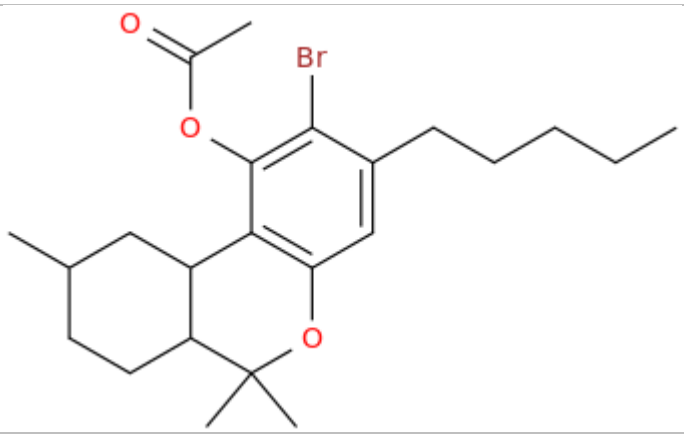
ANALYTICAL REPORT

2Br-HHC-O (C23H33BrO3)

2-bromo-6,6,9-trimethyl-3-pentyl-6H,6aH,7H,8H,9H,10H,10aH-benzo[c]isochromen-1-yl acetate

Remark – other NPS detected: none

Sample ID:	3324-25
Sample description:	liquid
Sample type:	synthesized /NFL- purchasing
Date of entry (DD/MM/YYYY) into NFL database:	22/08/2025
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	2-bromo-6,6,9-trimethyl-3-pentyl-6H,6aH,7H,8H,9H,10H,10aH-benzo[c]isochromen-1-yl acetate
Other names	2-bromo-heksahidrokanabinol acetat
Formula (per base form)	C23H33BrO3
M_w (g/mol)	437,42
Salt form/anions detected	base
StdInChIKey (per base form)	CISPFEQXHGXYRW-UHFFFAOYSA-N
Other NPS detected	none
Additional info (purity..)	the sample consists of accompanyng impurities, stereoisomers, etc.

[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

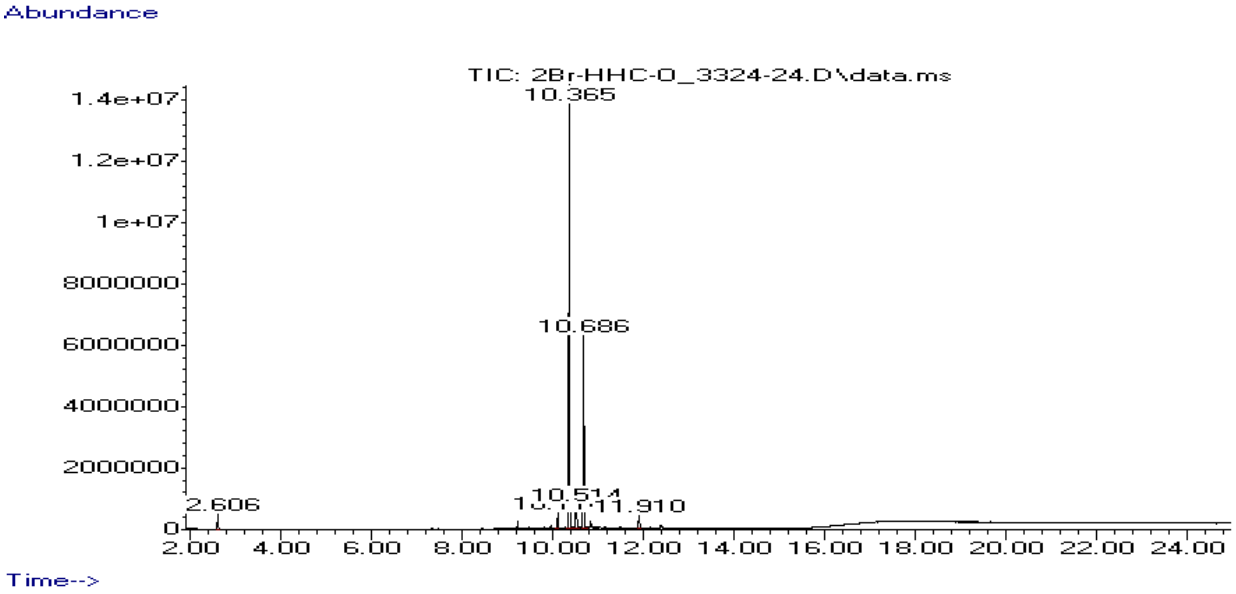
Supporting information

Solubility in	result/remark
CH_2Cl_2	soluble
MeOH	soluble
H_2O	not soluble

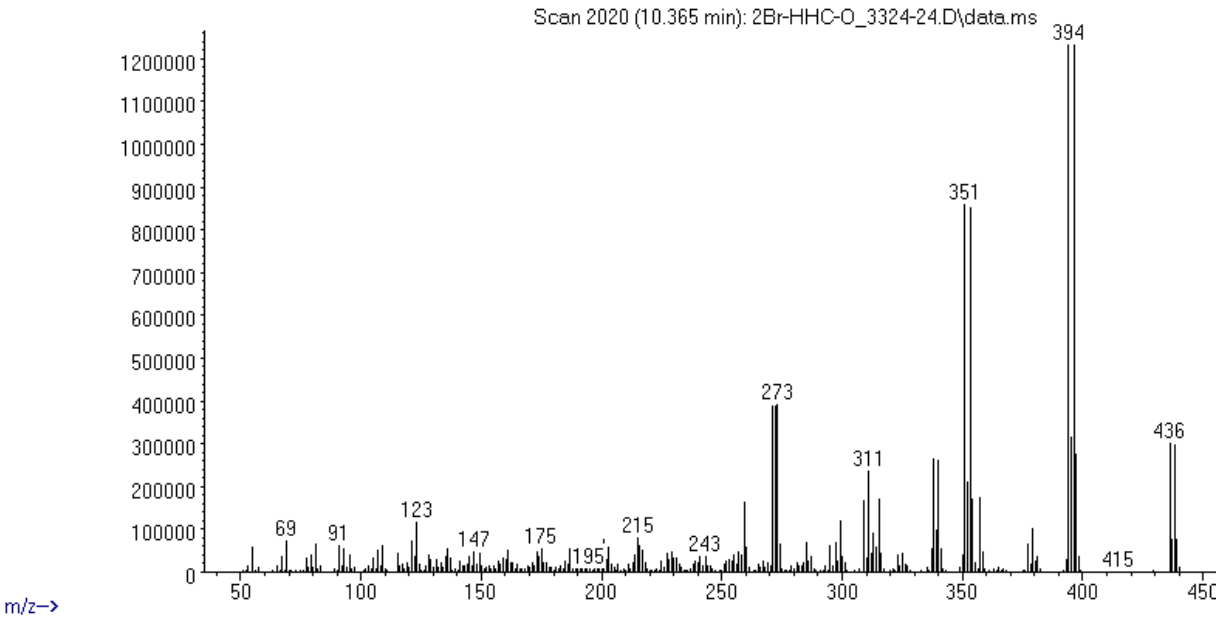
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 10,37 (refers to the most intensive peak) BP(1): 394; BP(2): 396,BP(3) :351,
HPLC-TOF	+	Exact mass (theoretical): 436,1613; measured value Δppm:-2,37; formula:C23H33BrO3
FTIR-ATR	+	direct measurement (sample as received)
FTIR (solid phase) always as base form	+	
IC (anions)		
NMR (in FKKT)	+	
validation		
other		

ANALYTICAL RESULTS

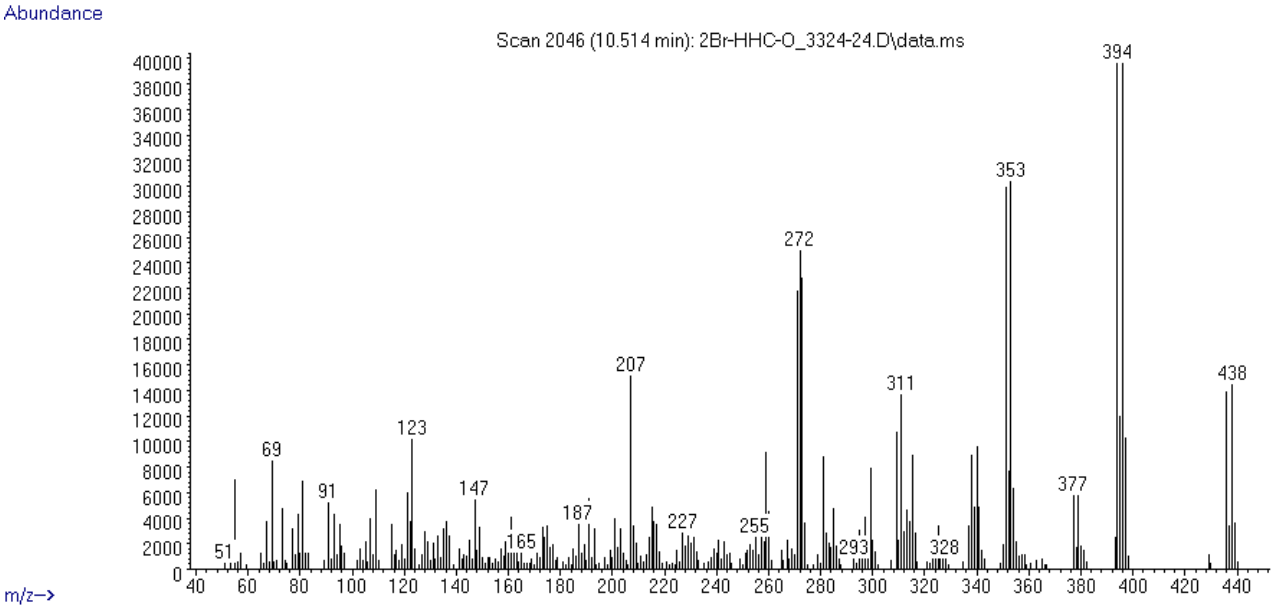
Chromatogram (GC)



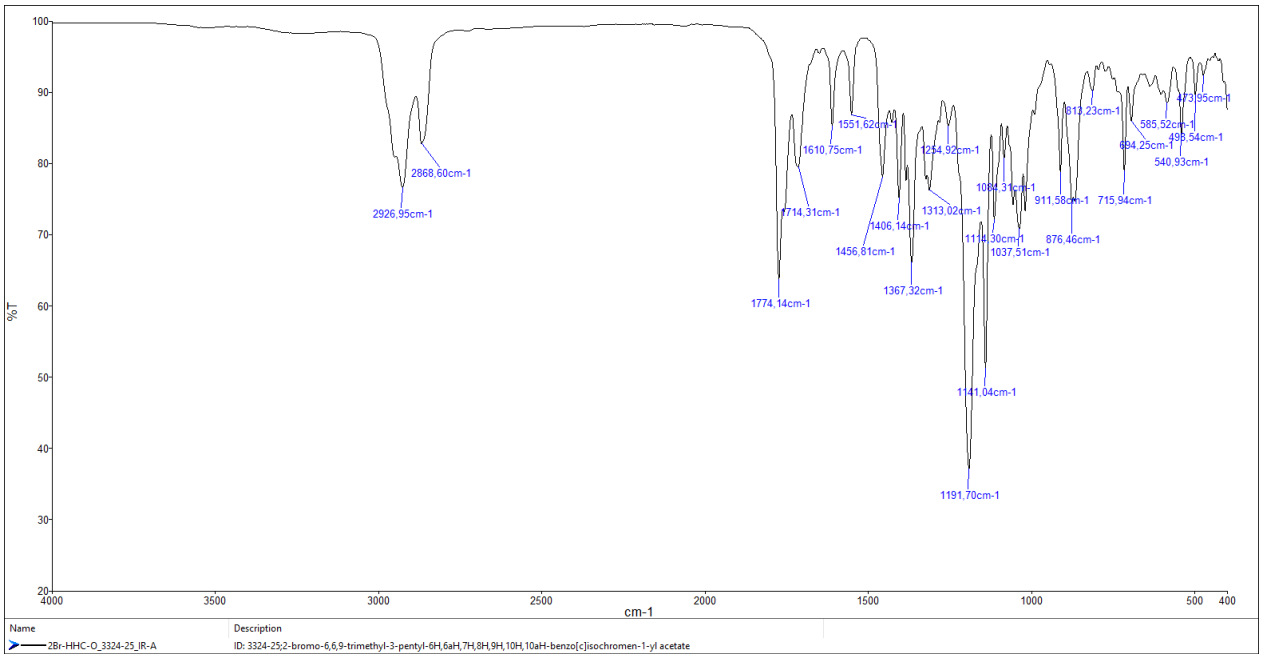
MS (EI): RT=10,365



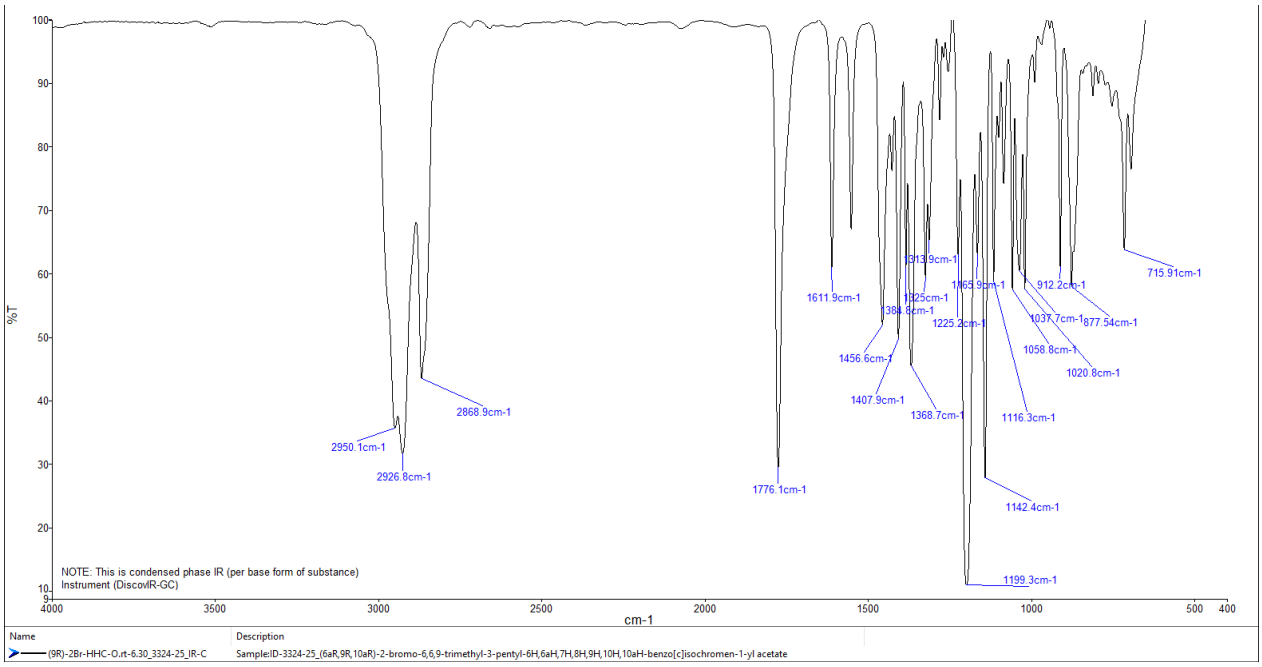
MS (EI): RT=10,514



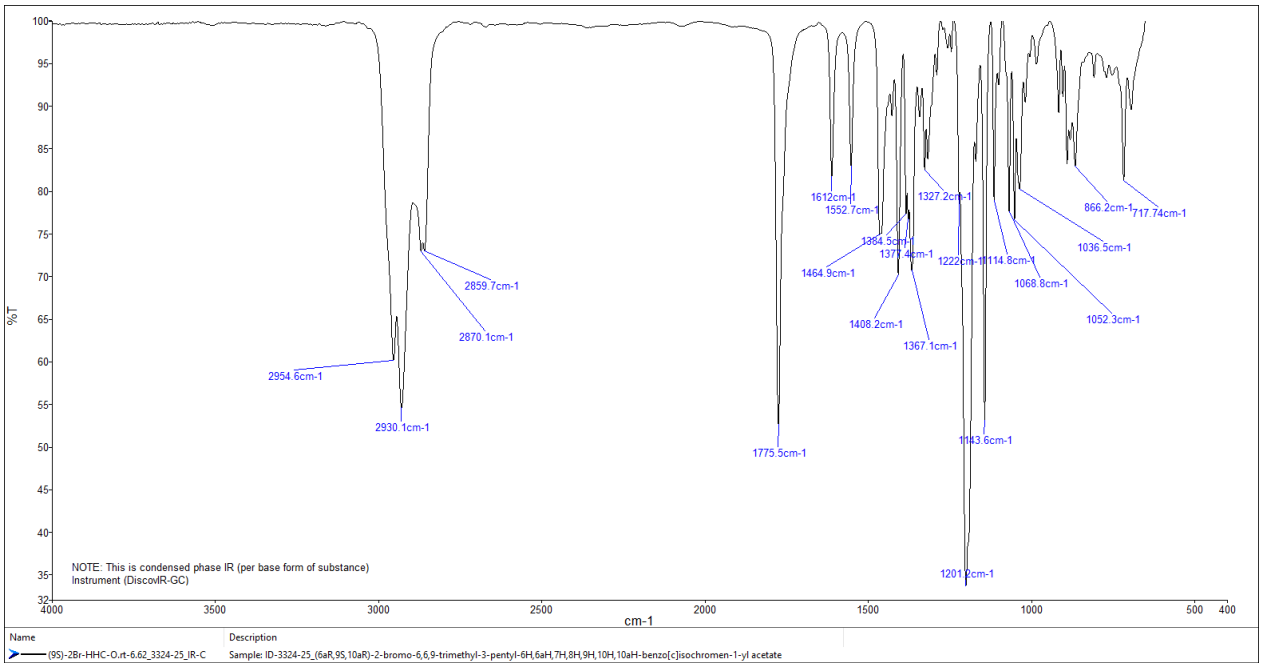
FTIR-ATR - direct measurement (sample as received)



IR (solid phase – after chromatographic separation at RT 1)



IR (solid phase – after chromatographic separation at RT 2)



TOF REPORT

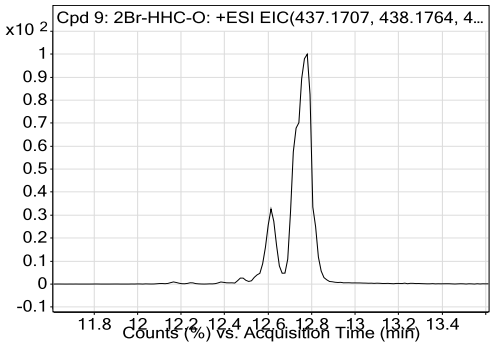
Data File	2Br-HHC-O_3324-25.d	**Sample Name**	ID 3324-25
Sample Type	Sample	**Position**	P1-A7
Instrument Name	6230B TOF LC-MS	**User Name**	TG
Acq Method	general-20_08_2024-XDB-C18-ESI+.m	**Acquired Time**	6/26/2025 10:05:45 AM
IRM Calibration Status	Success	**DA Method**	0-NPS in sorodne snovi.m
Comment	extract in MeOH		

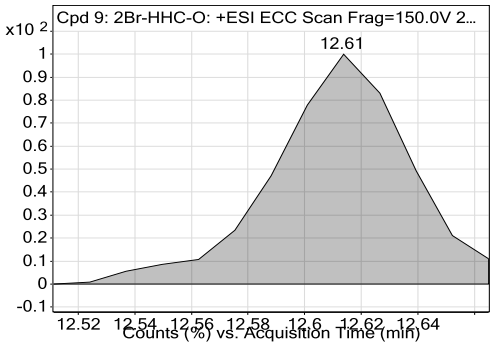
Compound Table

Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 9: 2Br-HHC-O	2Br-HHC-O	C23 H33 Br O3	12.61	436.1623

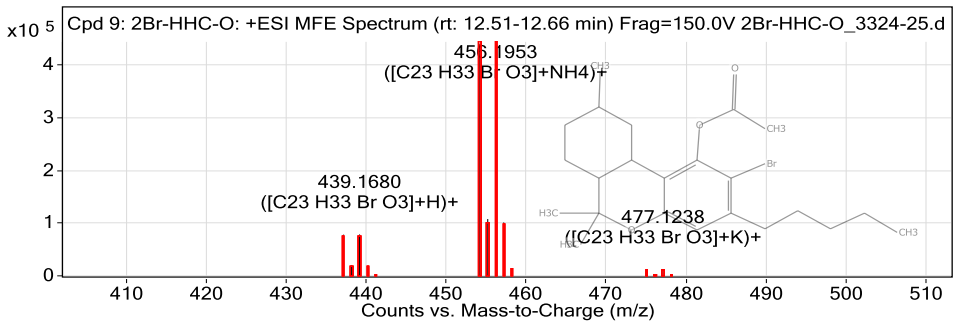
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
2Br-HHC-O	454.1969	12.61	436.1623	12.61	C23 H33 Br O3	436.1613	-2.37

Compound Chromatograms

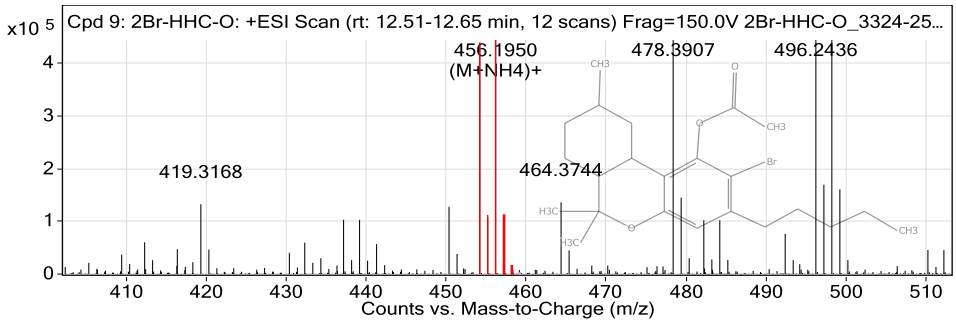




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
437.1694	1	78140.51	C23 H33 Br O3	(M+H)+
438.1726	1	19996.88	C23 H33 Br O3	(M+H)+
439.168	1	78552.55	C23 H33 Br O3	(M+H)+
440.1707	1	14052.48	C23 H33 Br O3	(M+H)+
454.1969	1	439479.82	C23 H33 Br O3	(M+NH4)+
455.1998	1	107760.21	C23 H33 Br O3	(M+NH4)+
456.1953	1	443855.53	C23 H33 Br O3	(M+NH4)+
457.1982	1	101220.02	C23 H33 Br O3	(M+NH4)+
458.2016	1	14569.61	C23 H33 Br O3	(M+NH4)+
477.1238	1	11982.2	C23 H33 Br O3	(M+K)+

--- End Of Report ---

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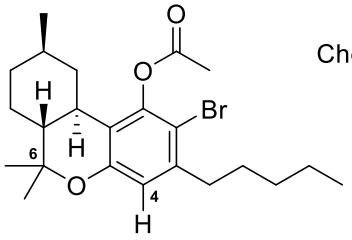
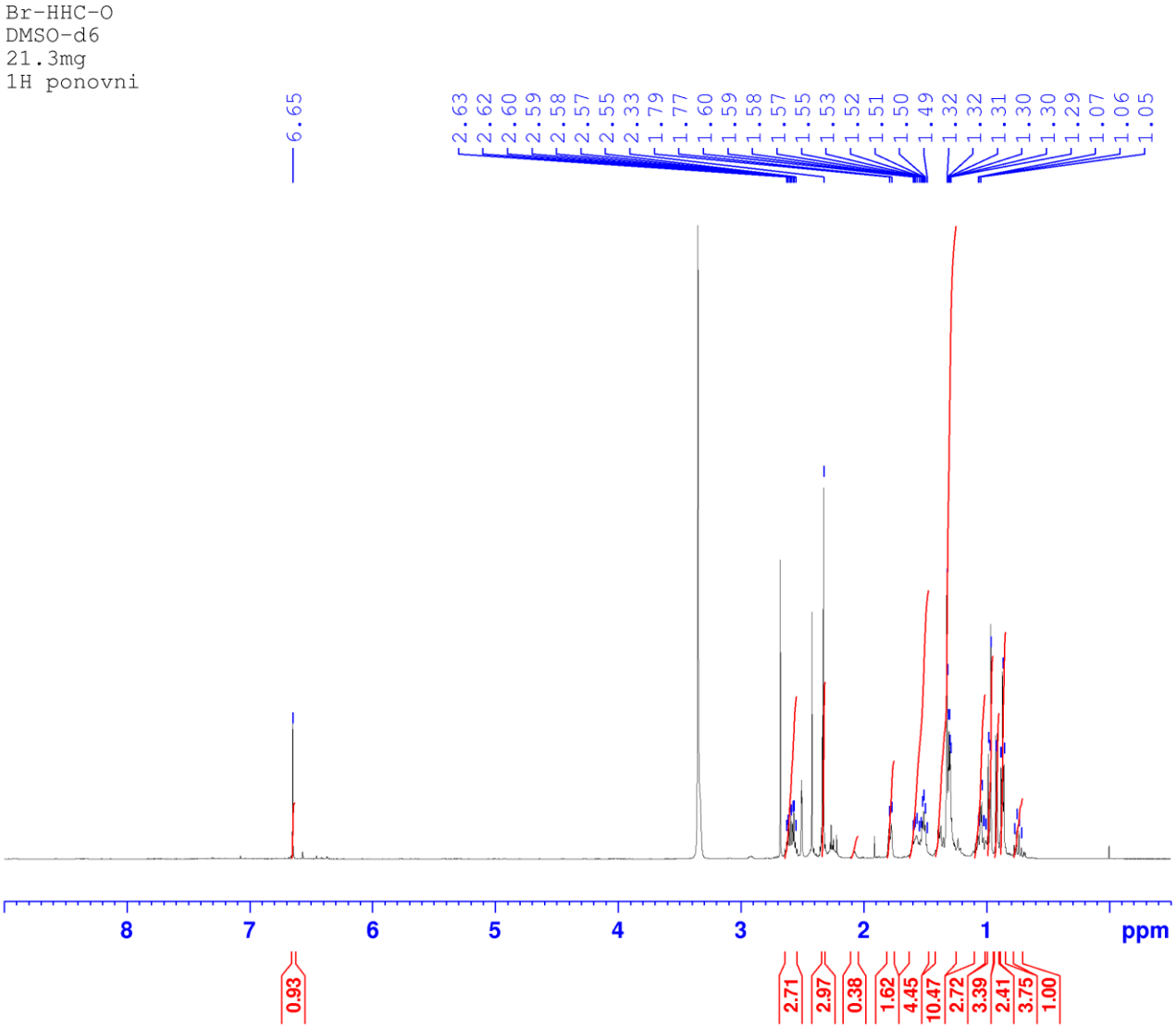
University
of Ljubljana

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:	**Br-HHC-O**
Received date:	April 15, 2025
Our notebook code:	Br-HHC-O
NMR sample preparation:	21.3 mg dissolved in 0.6 mL DMSO-d_6
NMR experiments:	^{1}H, ^{13}C, ^{1}H–^{1}H *gs*-COSY, ^{1}H–^{1}H *gs*-NOESY, ^{1}H–^{13}C *gs*-HSQC, ^{1}H–^{13}C *gs*-HMBC, ^{13}C DEPT-45, ^{13}C DEPT-90, ^{13}C DEPT-135
Proposed structure with formula, exact mass, molecular weight:	 Chemical Formula: $C_{23}H_{33}BrO_3$ Exact Mass: 436,16 Molecular Weight: 437,42
Chemical name:	(6a*R*, 9*R*, 10a*R*)-2-bromo-6,6,9-trimethyl-3-pentyl-6a,7,8,9,10,10a-hexahydro-6*H*-benzo[*c*]chromen-1-yl acetate
Comments:	- Structure elucidation based on 1D and 2D NMR spectra and HRMS. - The sample consists of accompanying impurities, stereoisomers, etc. - The position of bromine on the aromatic ring was determined based on NOE between C4-H and C6-C$\underline{H}_3$.
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:	April 25, 2025

Br-HHC-O
DMSO-d6
21.3mg
1H ponovni

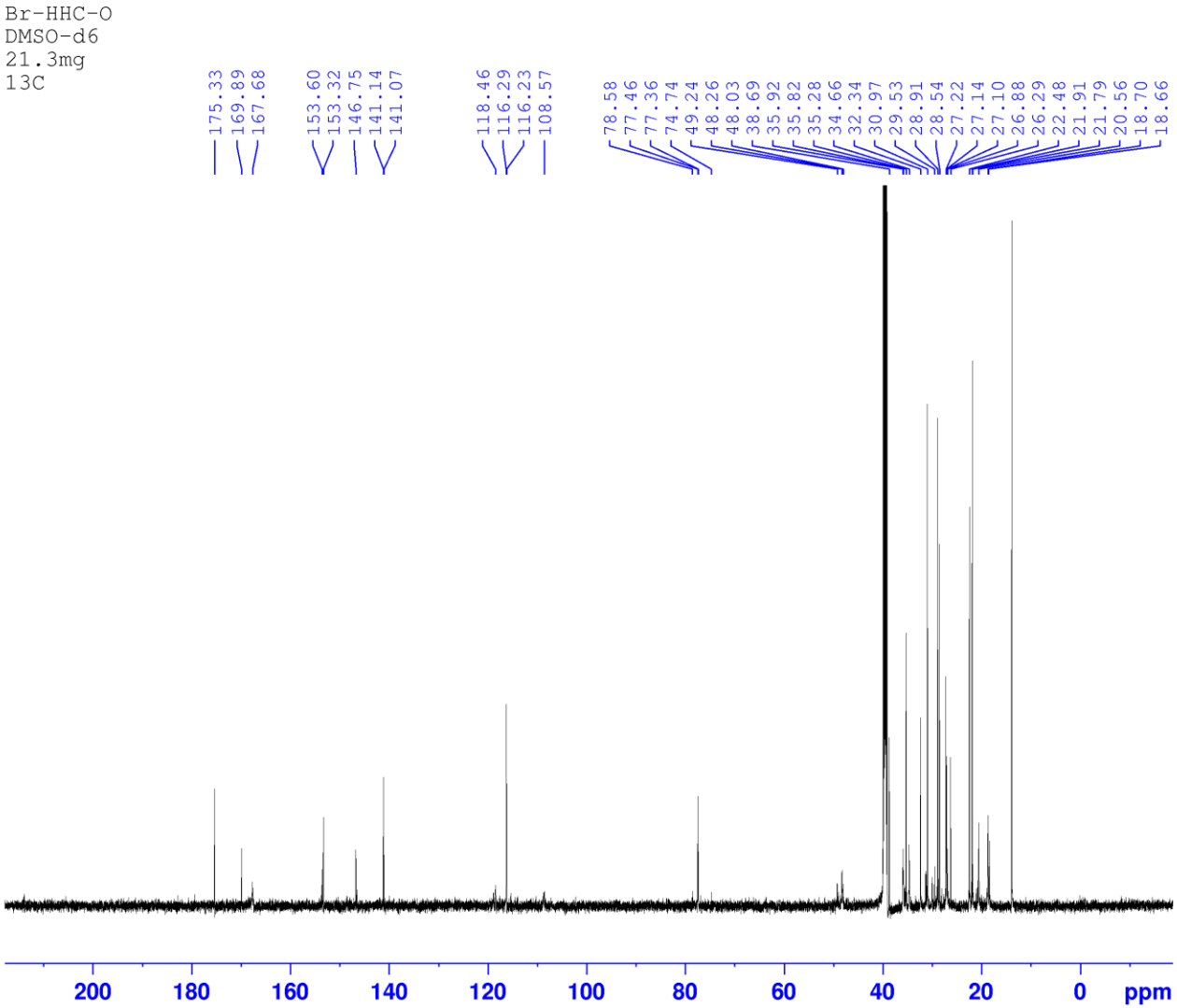


Current Data Parameters
NAME Br-HHC-O
EXPNO 18
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250415
Time 19.23 h
INSTRUM AV600 NEO
PROBHD Z176567_0002 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 11904.762 Hz
FIDRES 0.363304 Hz
AQ 2.7525120 sec
RG 53.3333
DW 42.000 usec
DE 8.79 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.82900047 W

F2 - Processing parameters
SI 65536
SF 600.1300015 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Br-HHC-O
DMSO-d6
21.3mg
13C



Current Data Parameters
NAME Br-HHC-O
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
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Time 17.22 h
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
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 296.1 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 112.23999786 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 70.00 usec
PLW2 19.82900047 W
PLW12 0.40495440 W
PLW13 0.20296310 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40