

ANALYTICAL REPORT

HHC-C9 (C25H40O2)

6,6,9-trimethyl-3-nonyl-6H,6aH,7H,8H,9H,10H,10aH-benzo[c]isochromen-1-olRemark – other NPS detected: **none**

Sample ID:	3327-25
Sample description:	crystalline
Sample type:	seized /LJ
Date of entry (DD/MM/YYYY) into NFL database:	03/09/2025
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	6,6,9-trimethyl-3-nonyl-6H,6aH,7H,8H,9H,10H,10aH-benzo[c]isochromen-1-ol
Other names	9(S)-Hexahydrocannabinol-C9 hexahydrocannabinol-C9 CC9
Formula (per base form)	C25H40O2
M _w (g/mol)	372,59
Salt form/anions detected	base
StdInChIKey (per base form)	IEJDLTWSCOMFKC-UHFFFAOYSA-N
Other NPS detected	none
Additional info (purity..)	90% of the compound based on 1H NMR spectrum

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 μ l and split mode (1:50). Injector temperature: 280 °C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 μ m. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 190 °C at rate 8 °C/min, then heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, then heating at 50 °C/min up to 325 °C and finally 9.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadropole temperatures 280°C and 180°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 μ l. 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 μ l and split mode (1:5). Injector temperature 280 °C. Chromatographic separation as above **(1)**. Split MS : IR = 1: 9.

MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.

IR (condensed (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 μ l

Supporting information

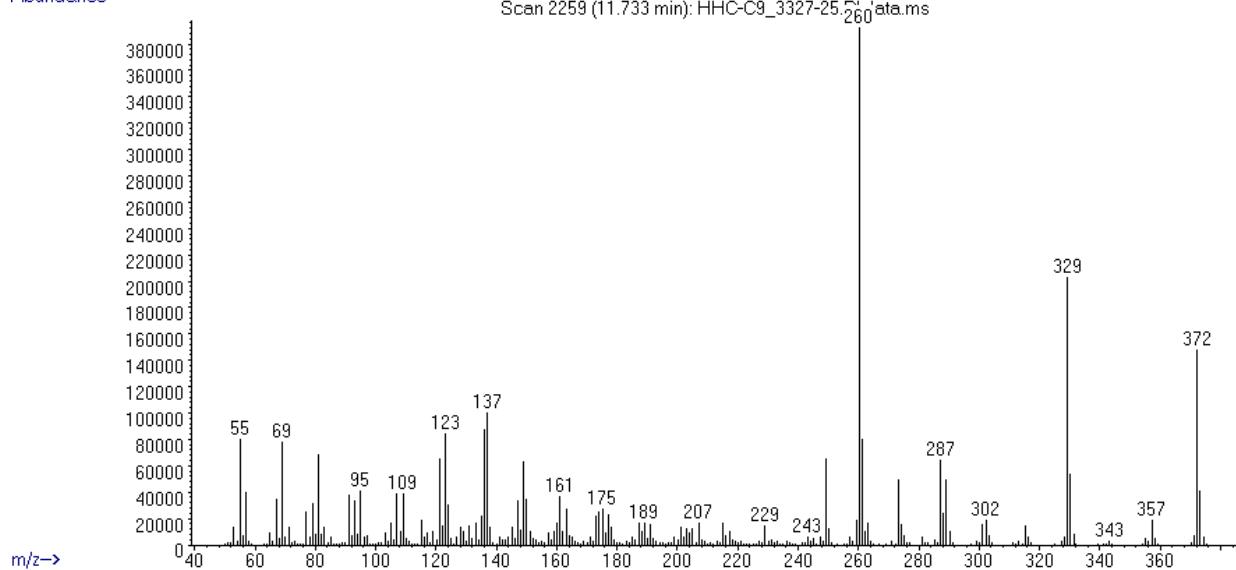
Solubility in	result/remark
CH ₂ Cl ₂	not soluble
MeOH	/
H ₂ O	soluble

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 11,73 BP(1): 260; BP(2): 329,BP(3) :372,
HPLC-TOF	+	Exact mass (theoretical): 372,3028; measured value Δppm:-4,24; formula:C25H40O2
FTIR-ATR	+	direct measurement (sample as received)
FTIR (solid phase) always as base form	+	
IC (anions)		
NMR (in FKKT)	+	
validation		
other		

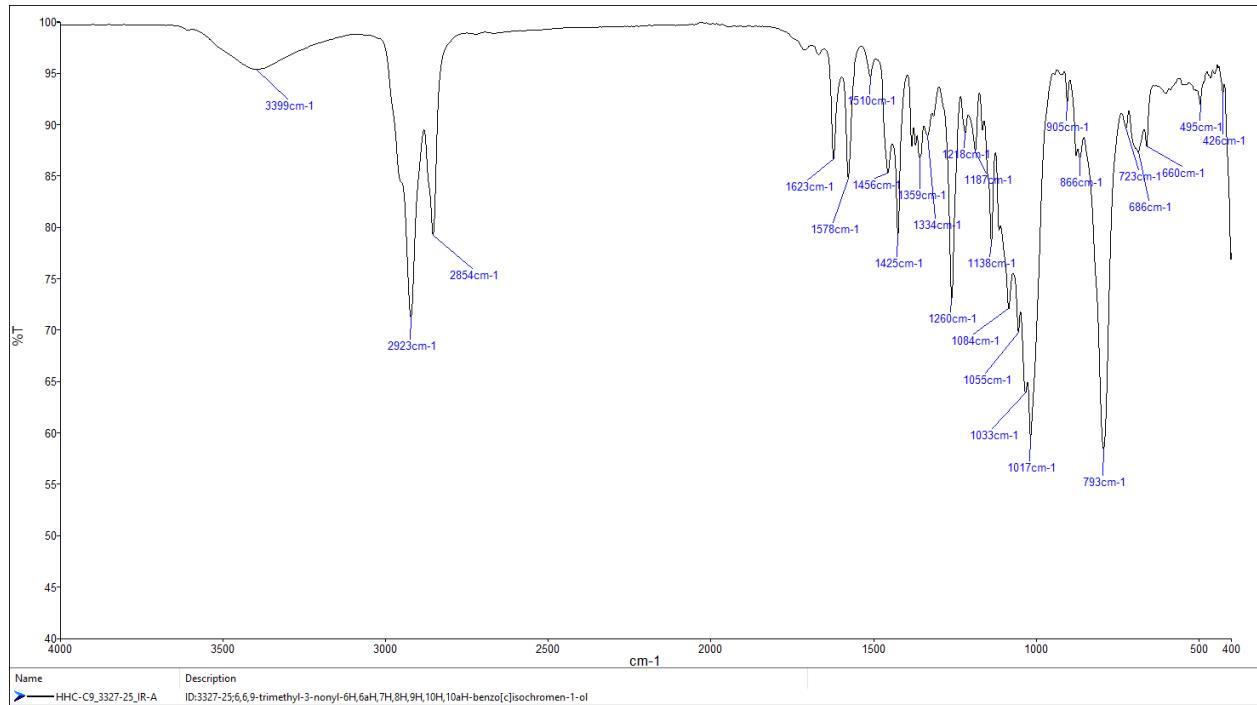
ANALYTICAL RESULTS

MS (EI)

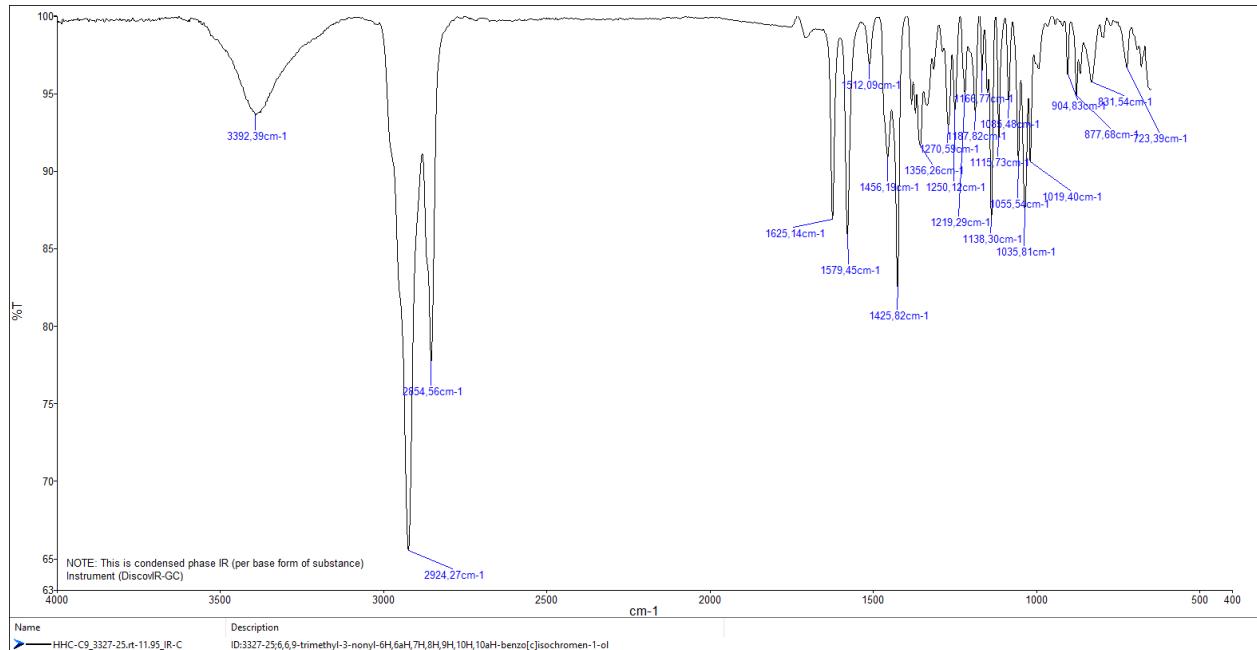
Abundance



FTIR-ATR - direct measurement (sample as received)



IR (solid phase – after chromatographic separation)



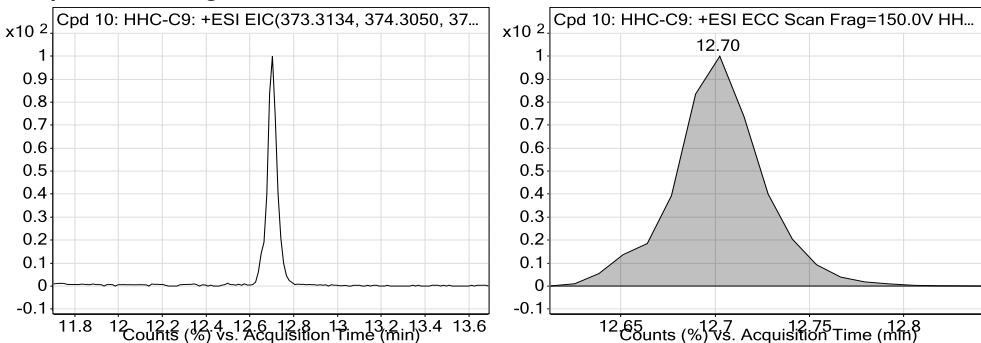
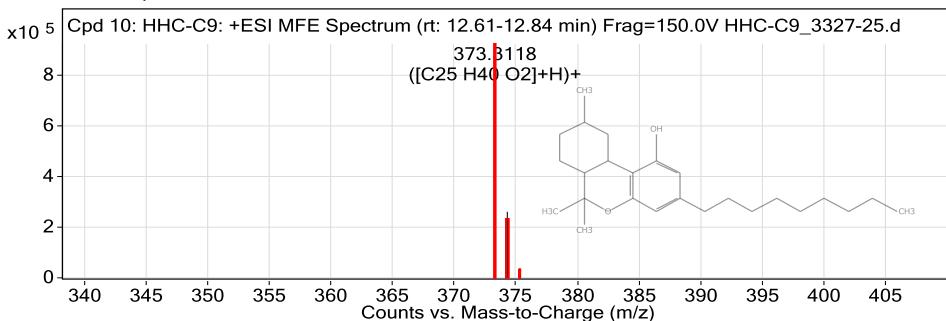
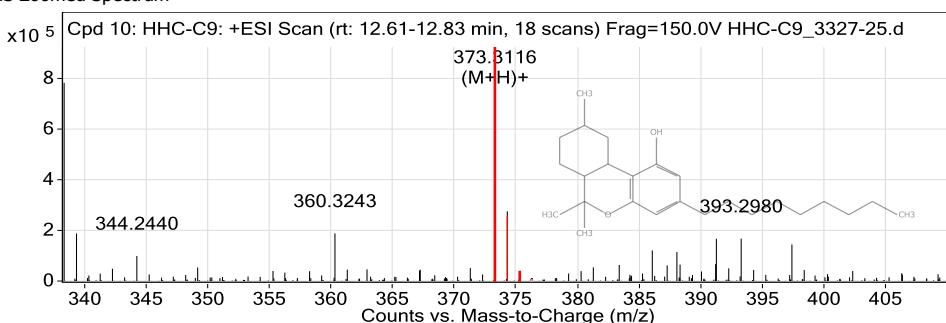
TOF REPORT

Data File	HHC-C9_3327-25.d	Sample Name	233-2871-25_1
Sample Type	Sample	Position	P1-A3
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	general-20_08_2024-XDB-C18-ESI+.m	Acquired Time	5/30/2025 10:25:33 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 10: HHC-C9	HHC-C9	C25 H40 O2	12.7	372.3044

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
HHC-C9	373.3118	12.7	372.3044	12.71	C25 H40 O2	372.3028	-4.24

Compound Chromatograms

MFE MS Zoomed Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
373.3118	1	921207.5	C25 H40 O2	$(M + H)^+$
374.3148	1	260153.13	C25 H40 O2	$(M + H)^+$
375.3168	1	36566.61	C25 H40 O2	$(M + H)^+$

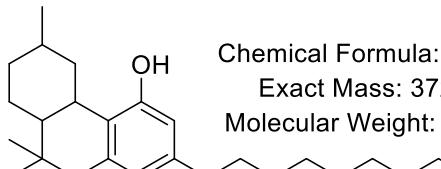
--- End Of Report ---

*Vecna pot 113
P. O. Box 537
SI-1001 Ljubljana
Slovenia
Phone: +386 1 479 8558
janez.kosmrlj@fkkt.uni-lj.si*

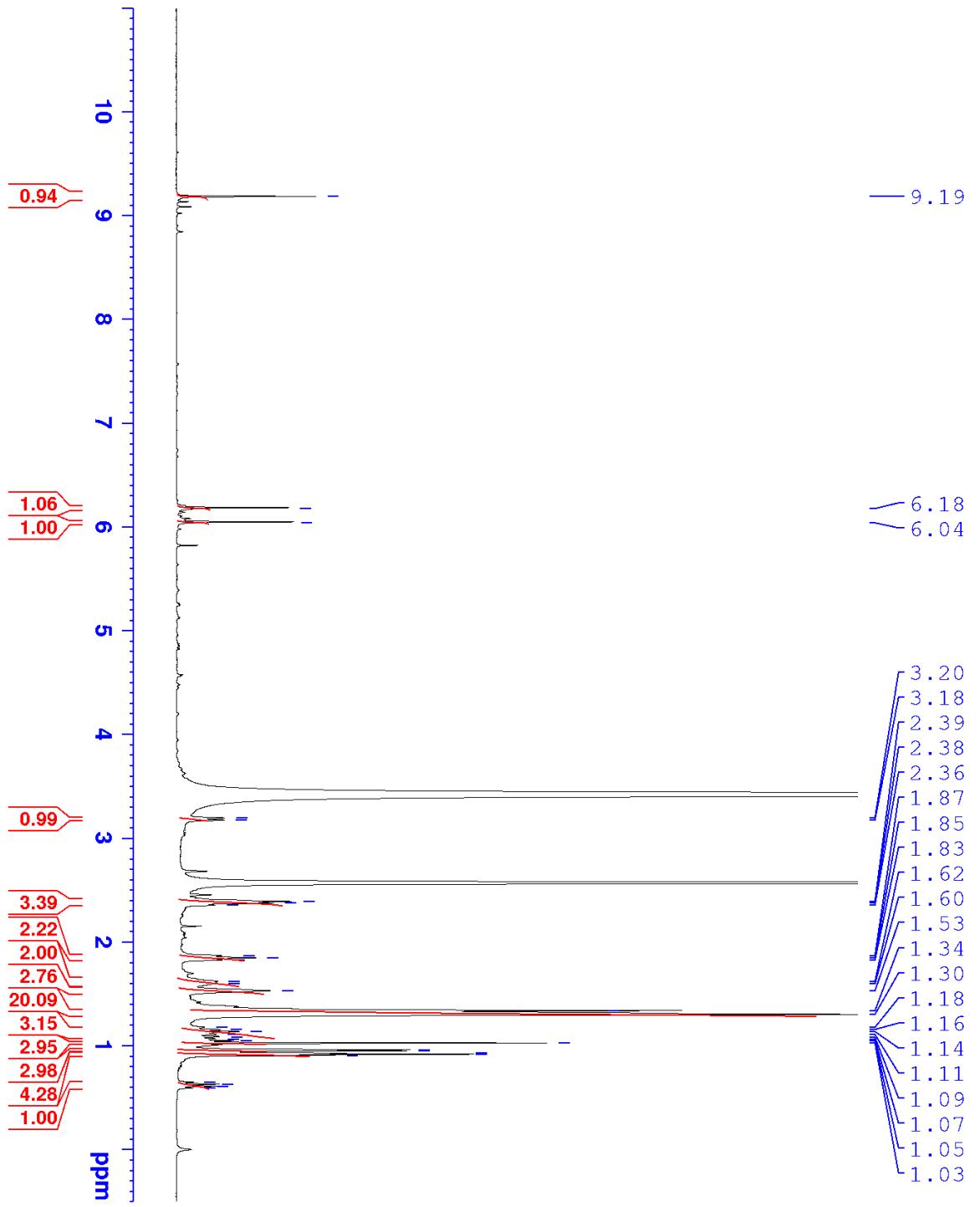
*University
of Ljubljana
Faculty of Chemistry
and Chemical Technology*



R E P O R T

Contract No.	C1714-21-460153 (Republic of Slovenia, Ministry of the Interior, POLICE)
Sample ID:	3327-25
Received date:	June 4, 2025
Our notebook code:	NFL-233-2871-2025-1
NMR sample preparation:	2 mg dissolved in 0.6 mL DMSO- <i>d</i> 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:	 <p>Chemical Formula: C₂₅H₄₀O₂ Exact Mass: 372,3028 Molecular Weight: 372,5930</p>
Chemical name:	3-nonyl-6a,7,8,9,10,10a-hexahydro-6,6,9-trimethyl-6H-dibenzo[b,d]pyran-1-ol
Comments:	- Structure elucidation based on 1D and 2D NMR spectra and HRMS. - The sample contains ca. 90% of the title compound 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:	June 12, 2025

NFL-233-2871-2025 1
1h
dmsO



Current Data Parameters
NAME NFL-233-2871-2025 1
EXPNO 40
PROCNO 1
F2 - Acquisition Parameters
Date_ 2025/6/11
Time 2.35 h
INSTRUM AV600 NEO
PROBHD Z176567_0002 T
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 11904.762 Hz
FIDRES 0.343304 Hz
AQ 2.7525120 sec
RG 101
DW 42.000 usec
DE 8.79 usec
TE 296.2 K
D1 1.0000000 sec
TDO 1
SFO1 600.1337058 MHz
NUC1 1H
PO 3.33 usec
P1 10.00 usec
PLW1 19.82900047 W
F2 - Processing parameters
ST 65536
SF 600.1299620 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00



NFL-3291-24
DMSO
17.4 mg⁻¹
13C

189.41

172.60

148.11
139.39
135.87
131.22
129.67
128.95
128.13
127.31
120.74
119.94

44.16

21.90
15.38



Current Data Parameters
NAME NFL-3291-24
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date 20250519
Time 22.41 h
INSTRUM AV600 NEO
PROBHD Z176567_0002 (PULPROG zgppg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 35714.285 Hz
ETR 1.089913 Hz
AQ 0.9175040 sec
RG 101
DW 14.000 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 150.9178988 MHz
NUC1 13C
PO 4.00 usec
P1 12.00 usec
P1W1 112.23999786 W
SF02 600.1324005 MHz
NUC2 1H
CPDPRG[2
P1W2 70.00 usec
PLW12 19.82200047 W
PLW13 0.44495440 W
PLW13 0.20296310 W

waltz65
P1W2 19.82200047 W
PLW12 0.44495440 W
PLW13 0.20296310 W
F2 - Processing parameters
SI 32768
SF 150.9028950 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 ppm

