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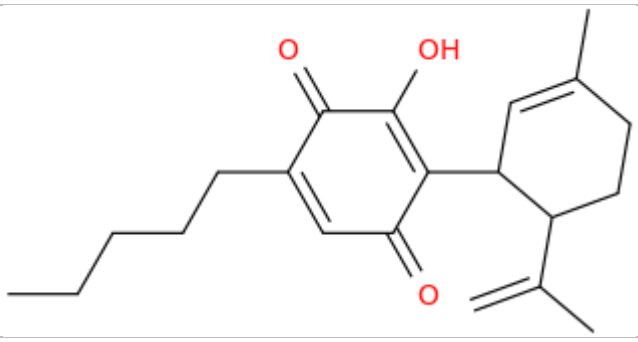
ANALYTICAL REPORT

HU-331 (C21H28O3)

6-hydroxy-3'-methyl-4-pentyl-6'-(prop-1-en-2-yl)-[1,1'-bi(cyclohexane)]-1(6),2',3-triene-2,5-dione

Remark – other NPS detected: none

Sample ID:	3290-24
Sample description:	powder
Sample type:	test purchase /NFL- purchasing
Date of entry (DD/MM/YYYY) into NFL database:	07/08/2025
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	6-hydroxy-3'-methyl-4-pentyl-6'-(prop-1-en-2-yl)-[1,1'-bi(cyclohexane)]-1(6),2',3-triene-2,5-dione
Other names	3-hydroxy-2-(6-isopropenyl-3-methyl-cyclohex-2-en-1-yl)-5-pentyl-1,4-benzoquinone; 3S,4R-p-benzoquinone-3-hydroxy-2-p-mentha-(1,8)-dien-3-yl-5-pentyl; Cannabidiol hydroxyquinone; Cannabidiolquinone; CBDHQ; CBDQ; VCE-004
Formula (per base form)	C21H28O3
M_w (g/mol)	328,45
Salt form/anions detected	base
StdInChIKey (per base form)	WDXXEUARVHTWQF-UHFFFAOYSA-N
Other NPS detected	none
Additional info (purity..)	95% purity of a sample 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 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

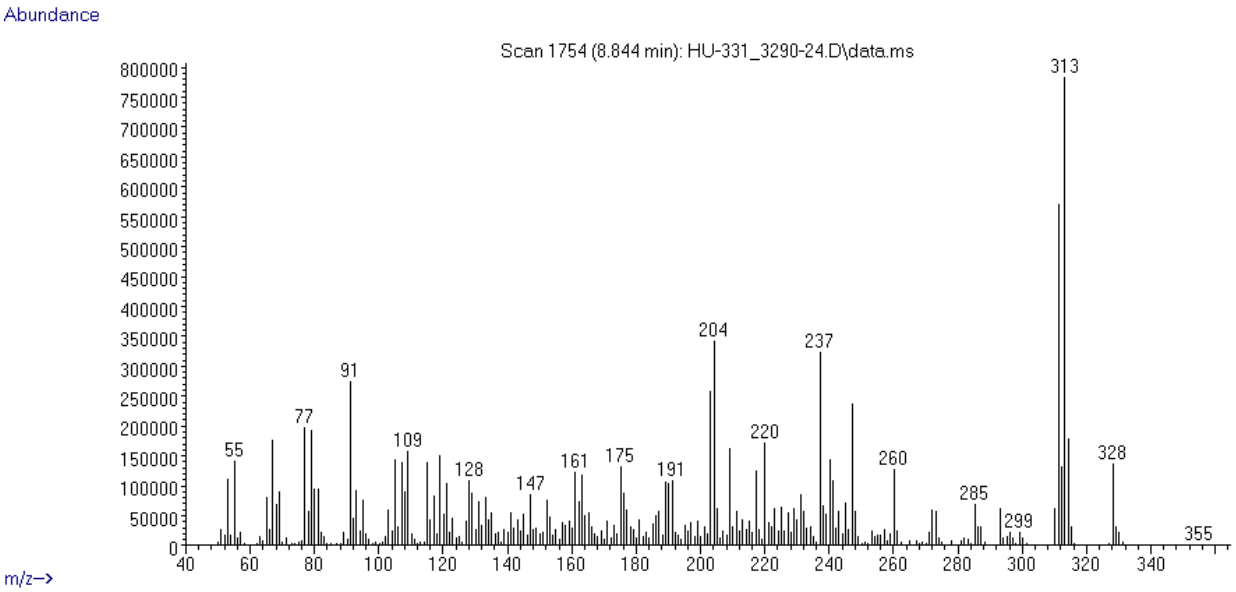
Supporting information

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

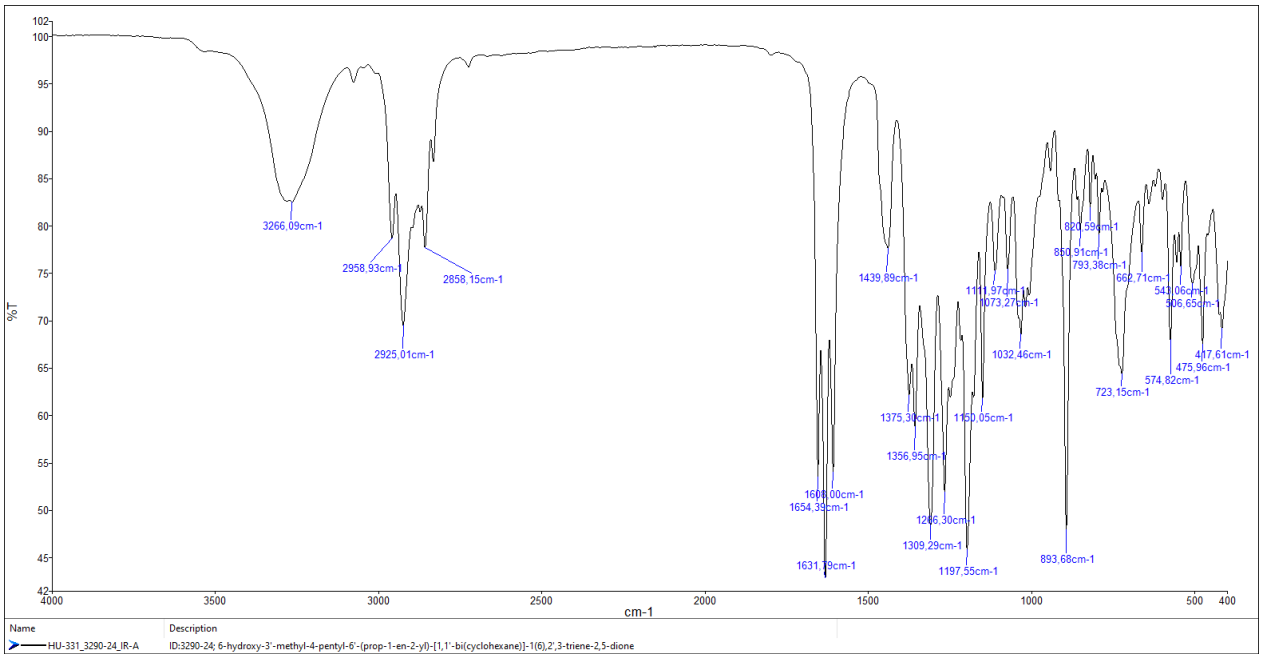
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 8,84 BP(1): 313; BP(2): 311,BP(3) :204,
HPLC-TOF	+	Exact mass (theoretical): 328,2038; measured value Δppm:-0,99; formula:C21H28O3
FTIR-ATR	+	direct measurement (sample as received)
FTIR (solid phase) always as base form	+	
IC (anions)	/	
NMR (in FKKT)	+	
validation		
other		

ANALYTICAL RESULTS

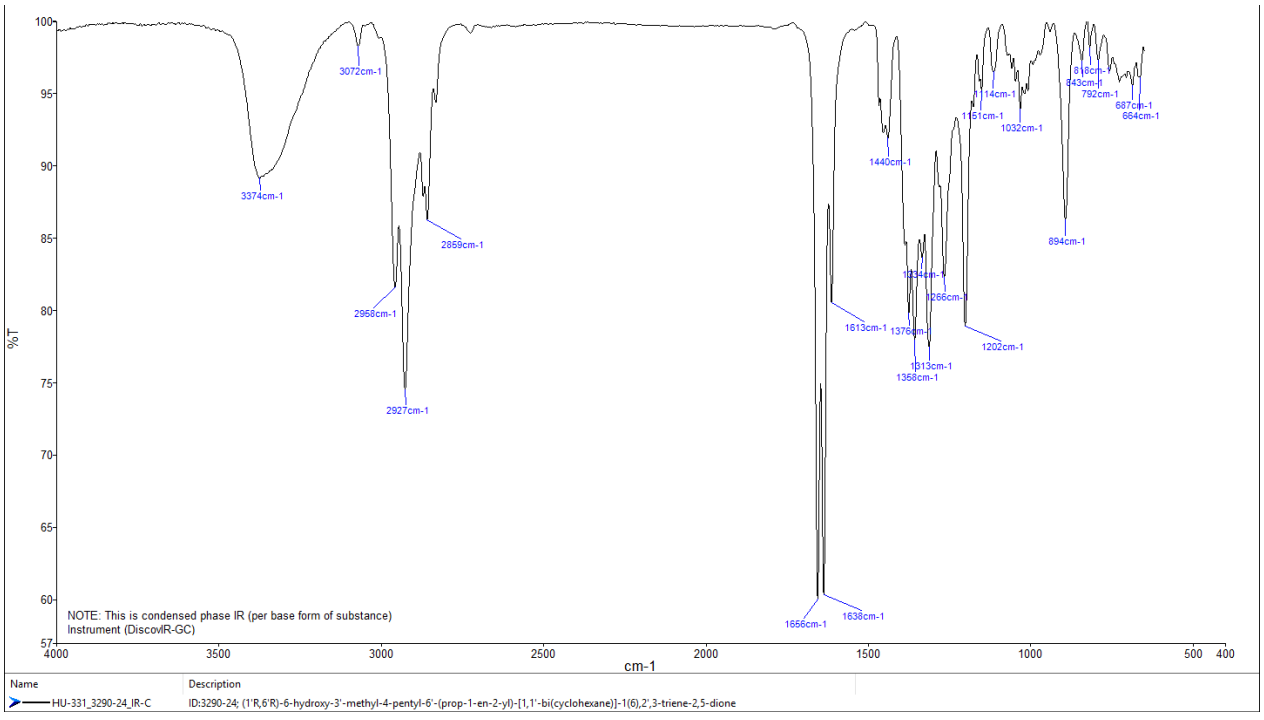
MS (EI)



FTIR-ATR - direct measurement (sample as received)



IR (solid phase – after chromatographic separation)



TOF REPORT

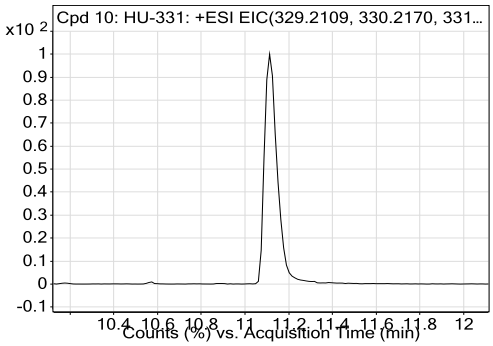
Data File	HU-331_3290-24.d	**Sample Name**	ID 3290-24
Sample Type	Sample	**Position**	P1-A6
Instrument Name	6230B TOF LC-MS	**User Name**	TG
Acq Method	general-01_08_2024-XDB-C18-ESI+.m	**Acquired Time**	8/8/2024 11:24:58 AM
IRM Calibration Status	Success	**DA Method**	0-NPS in sorodne snovi.m
Comment	extract in MeOH		

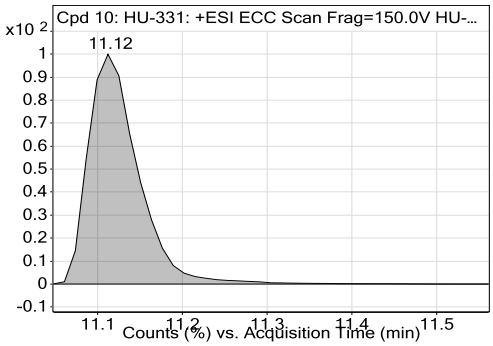
Compound Table

Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 10: HU-331	HU-331	C21 H28 O3	11.12	328.2042

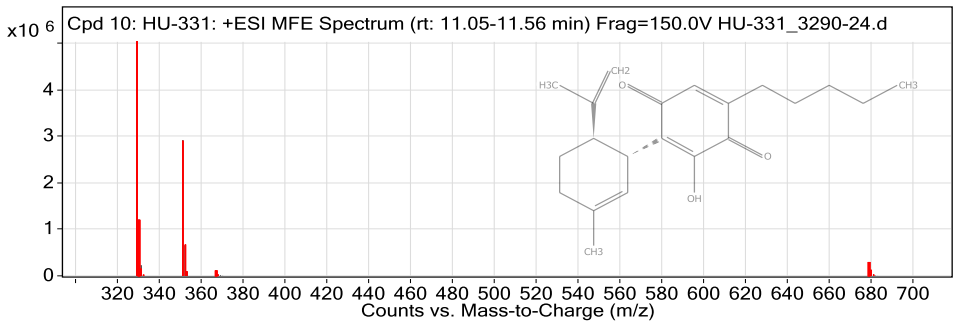
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
HU-331	329.2112	11.12	328.2042	11.12	C21 H28 O3	328.2038	-0.99

Compound Chromatograms

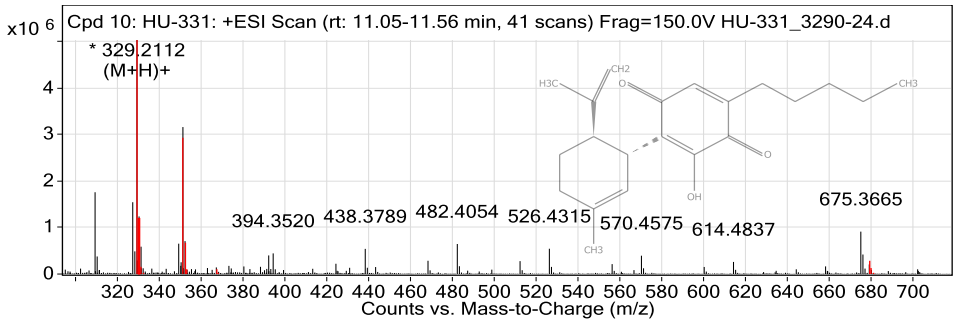




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
329.2112	1	5024272.5	C21 H28 O3	(M+H)+
330.2151	1	1207092.92	C21 H28 O3	(M+H)+
331.2117	1	228851.89	C21 H28 O3	(M+H)+
351.1933	1	2915881.75	C21 H28 O3	(M+Na)+
352.1972	1	657002.39	C21 H28 O3	(M+Na)+
353.1998	1	85482.45	C21 H28 O3	(M+Na)+
367.1677	1	104447.14	C21 H28 O3	(M+K)+
679.3976	1	278155.19	C21 H28 O3	(2M+Na)+
680.4014	1	124430.19	C21 H28 O3	(2M+Na)+
681.4044	1	31154.28	C21 H28 O3	(2M+Na)+

--- End Of Report ---

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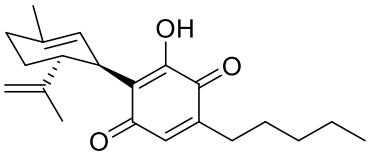
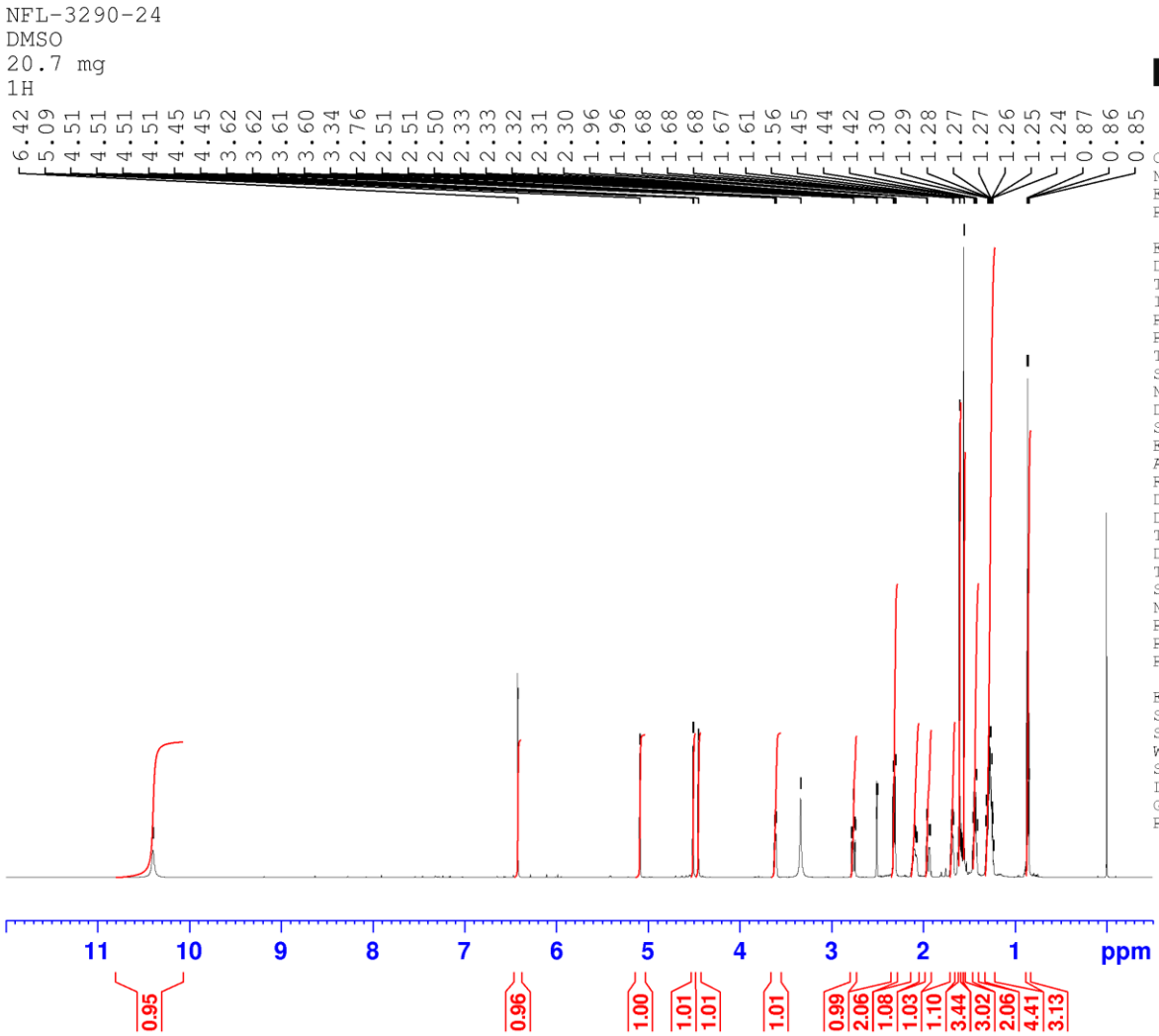
University
of Ljubljana

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:	**3290-24**
Received date:	May 19, 2025
Our notebook code:	NFL-3290-24
NMR sample preparation:	20.7 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: $C_{21}H_{28}O_3$ Exact Mass: 328,2038 Molecular Weight: 328,4520
Chemical name:	(1'*R*,6'*R*)-6-hydroxy-3'-methyl-4-pentyl-6'-(prop-1-en-2-yl)-[1,1'-bi(cyclohexane)]-2',3,6-triene-2,5-dione
Comments:	- Structure elucidation based on 1D and 2D NMR spectra, HRMS, optical activity {[α]$_D$: −111° (2 mg/mL in EtOH)} and comparison with the literature data {[α]$_D$: −110° (0.1 mg/mL in EtOH), reported by Kogan N.M., Rabinowitz R., Levi P., et al., *J. Med. Chem*. 2004, 47, 3800. - The sample contains ca. 95% 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:	May 26, 2025

NFL-3290-24
DMSO
20.7 mg
1H



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PROCNO 1

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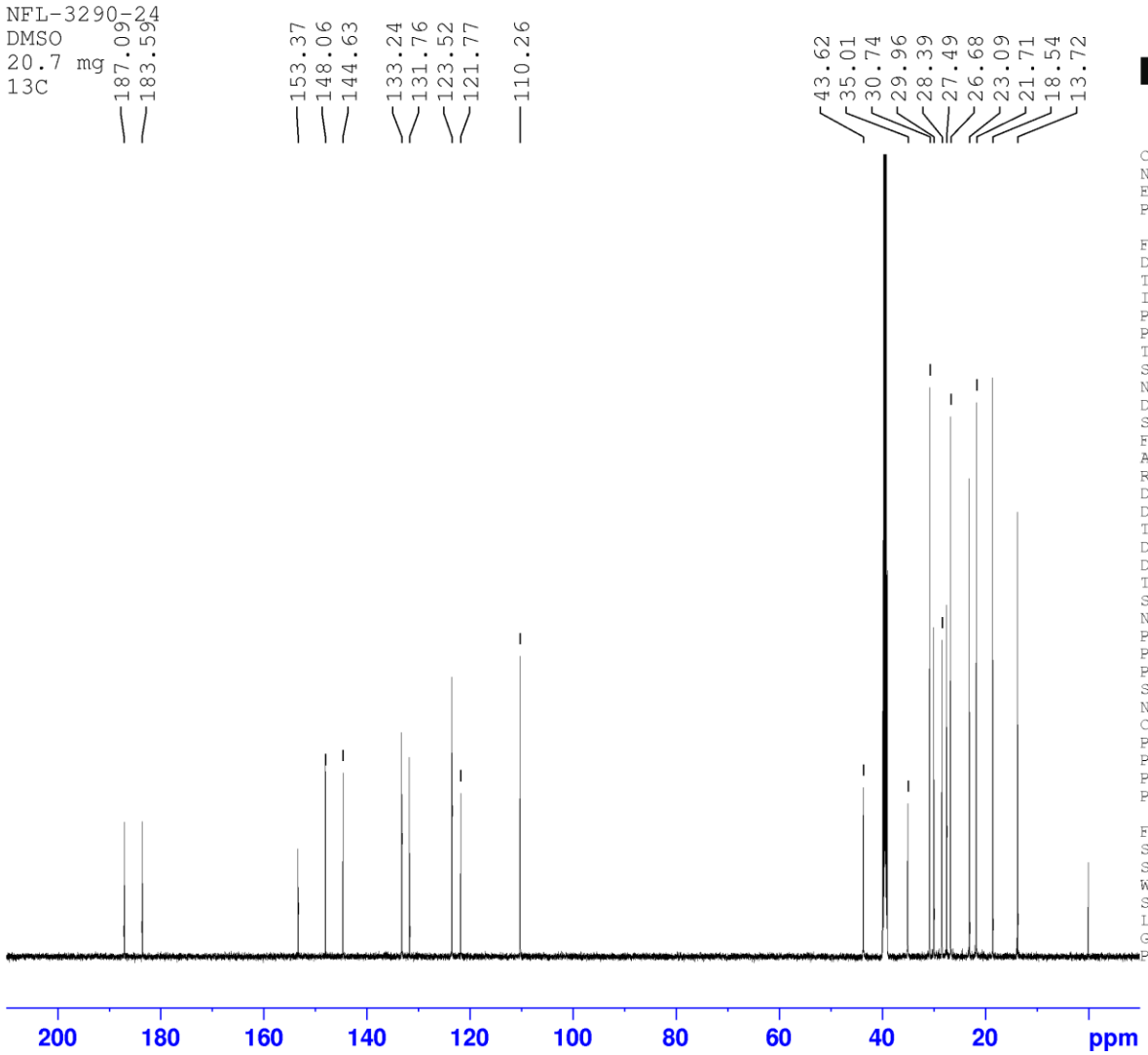
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 11904.762 Hz
FIDRES 0.363304 Hz
AQ 2.7525120 sec
RG 54.7368
DW 42.000 usec
DE 8.79 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.82900047 W

F2 - Processing parameters
SI 65536
SF 600.1300004 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NFL-3290-24
DMSO
20.7 mg
13C



BRUKER

Current Data Parameters
NAME NFL-3290-24
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
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Time 18.23 h
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PROBHD Z176567_0002 (
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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SF 150.9028929 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40