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NATIONAL FORENSIC LABORATORY
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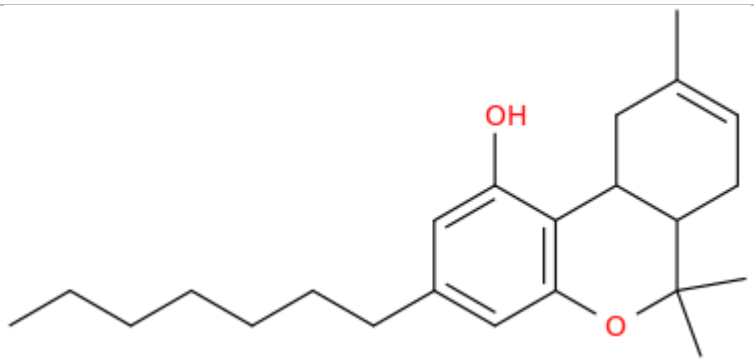
# ANALYTICAL REPORT

## delta-8-THCP (C23H34O2)

### 3-heptyl-6,6,9-trimethyl-6H,6aH,7H,10H,10aH-benzo[c]isochromen-1-ol

Remark – other NPS detected: none

| | |
|---|---|
| Sample ID: | 3227-22 |
| Sample description: | liquid |
| Sample type: | collected /Customs, Slovenia |
| Date of entry (DD/MM/YYYY) into NFL database: | 26/08/2024 |
| 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-heptyl-6,6,9-trimethyl-6H,6aH,7H,10H,10aH-benzo[c]isochromen-1-ol |
| Other names | 3-heptyl-6a,7,10,10a-tetrahydro-6,6,9-trimethyl-6H-dibenzo[b,d]pyran-1-ol ; JWH 091; Δ8-Tetrahydrocannabiphorol; Δ8-THC-C7; Δ8-THC-heptyl; 3-heptyl-6,6,9-trimethyl-6a,7,10,10a-tetrahydrobenzo[c]chromen-1-ol |
| Formula (per base form) | C23H34O2 |
| $M_w$ (g/mol) | 342,52 |
| Salt form/anions detected | base |
| StdInChIKey (per base form) | RGXKCMQANRHRCO-UHFFFAOYSA-N |
| Other NPS detected | none |
| Additional info (purity..) | 70% 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

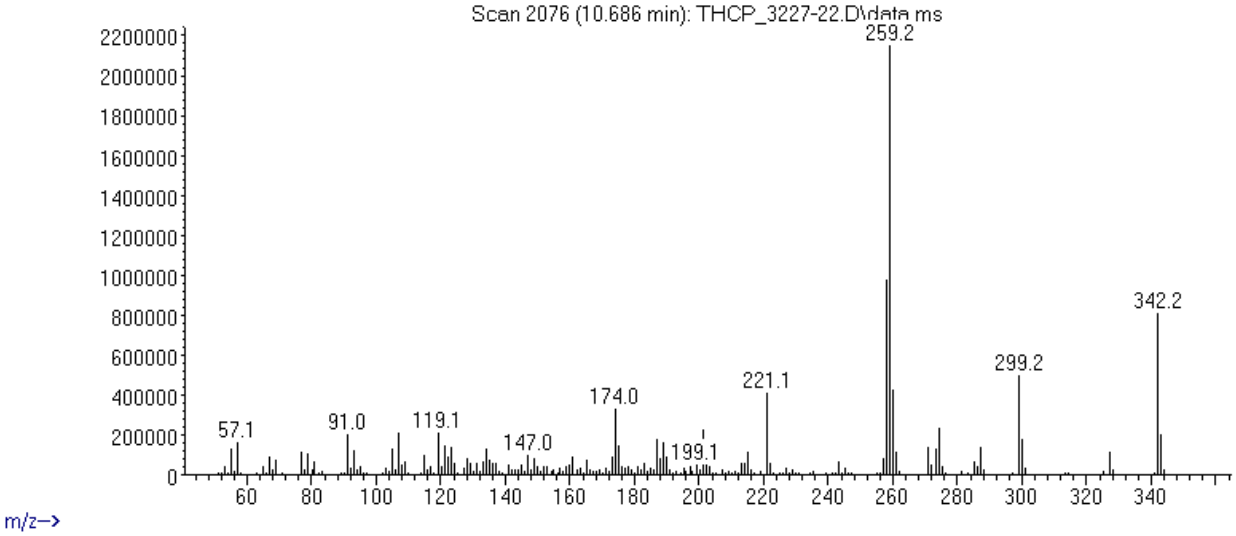
Supporting information

| Solubility in | result/remark |
|---|---|
| $CH_2Cl_2$ | |
| MeOH | |
| $H_2O$ | |

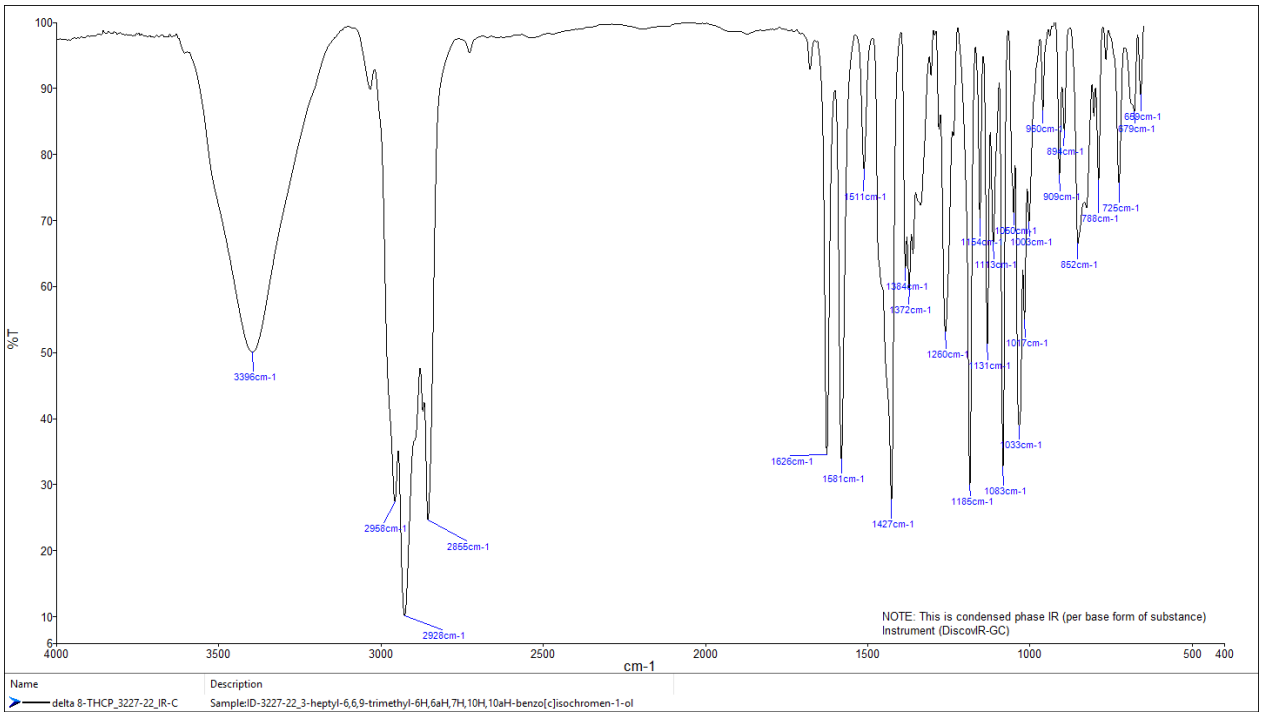
| Analytical technique: | applied | remarks |
|---|---|---|
| GC-MS (EI ionization) | + | NFL GC-RT (min): 10,69<br>BP(1): 259; BP(2): 258,BP(3) :342, |
| HPLC-TOF | + | Exact mass (theoretical): 342,2559;<br>measured value Δppm:-1,57;<br>formula:C23H34O2 |
| FTIR-ATR | - | direct measurement (sample 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

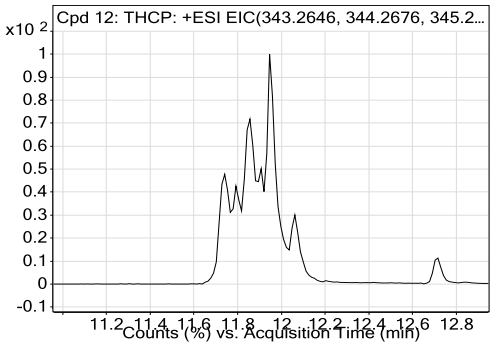
| | | | |
|---|---|---|---|
| **Data File** | THCp_3227_22.d | **Sample Name** | ID-3227-22 |
| **Sample Type** | Sample | **Position** | P1-A3 |
| **Instrument Name** | 6230B TOF LC-MS | **User Name** | TG |
| **Acq Method** | general-15_01_2020-XDB-C18-ESI+.m | **Acquired Time** | 12/28/2022 9:32:41 AM |
| **IRM Calibration Status** | Success | **DA Method** | 0-NPS in sorodne snovi.m |
| **Comment** | extract in MeOH | | |

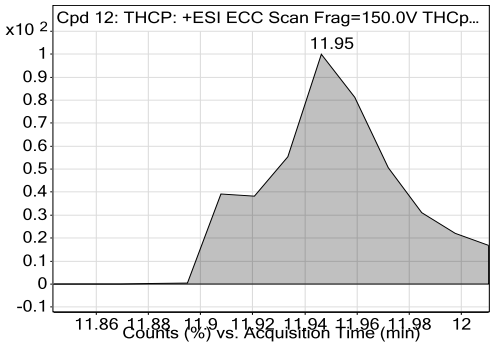
**Compound Table**

| Label | Compound Name | MFG Formula | Obs. RT | Obs. Mass |
|---|---|---|---|---|
| Cpd 12: THCP | THCP | C23 H34 O2 | 11.95 | 342.2564 |

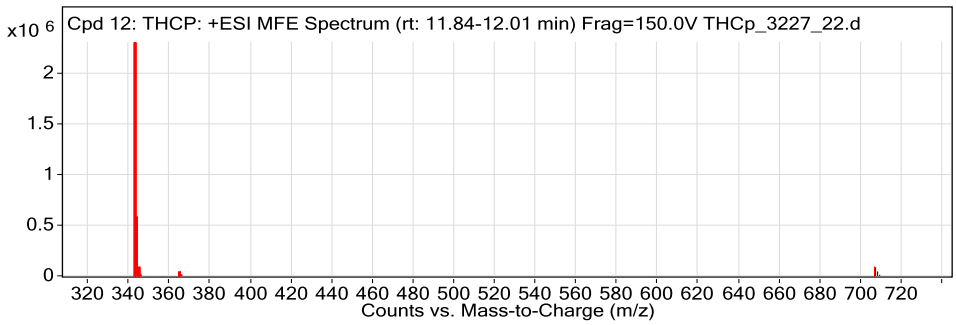
| Name | *Obs. m/z* | Obs. RT | Obs. Mass | DB RT | DB Formula | DB Mass | DB Mass Error (ppm) |
|---|---|---|---|---|---|---|---|
| **THCP** | 343.2643 | 11.95 | 342.2564 | 11.95 | C23 H34 O2 | 342.2559 | -1.57 |

**Compound Chromatograms**

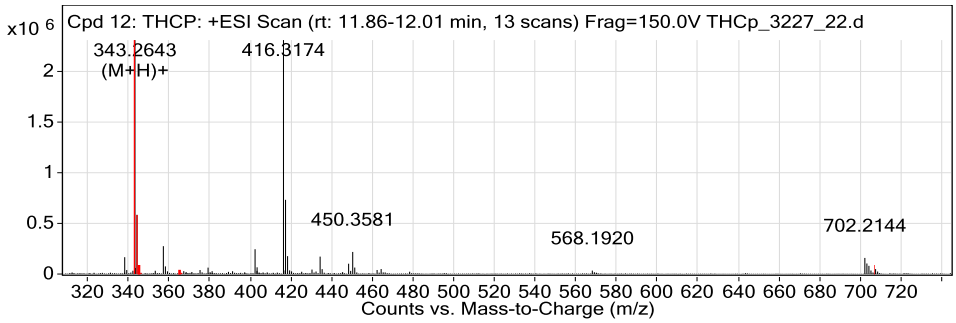



MFE MS Zoomed Spectrum




MS Zoomed Spectrum




**MS Spectrum Peak List**

| *Obs. m/z* | Charge | Abund | Formula | Ion/Isotope |
|---|---|---|---|---|
| 343.2643 | 1 | 2312088.75 | C23 H34 O2 | (M+H)+ |
| 344.268 | 1 | 585651.29 | C23 H34 O2 | (M+H)+ |
| 345.2707 | 1 | 66939.2 | C23 H34 O2 | (M+H)+ |
| 346.2715 | 1 | 2293.71 | C23 H34 O2 | (M+H)+ |
| 365.2467 | 1 | 35466.8 | C23 H34 O2 | (M+Na)+ |
| 366.2533 | 1 | 7452.59 | C23 H34 O2 | (M+Na)+ |
| 707.5015 | 1 | 84368.25 | C23 H34 O2 | (2M+Na)+ |
| 708.5052 | 1 | 44117.19 | C23 H34 O2 | (2M+Na)+ |
| 709.5074 | 1 | 11026.33 | C23 H34 O2 | (2M+Na)+ |

--- End Of Report ---

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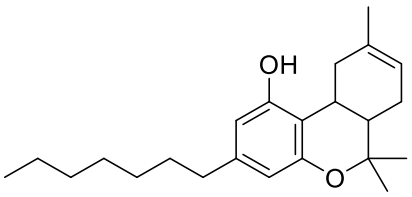
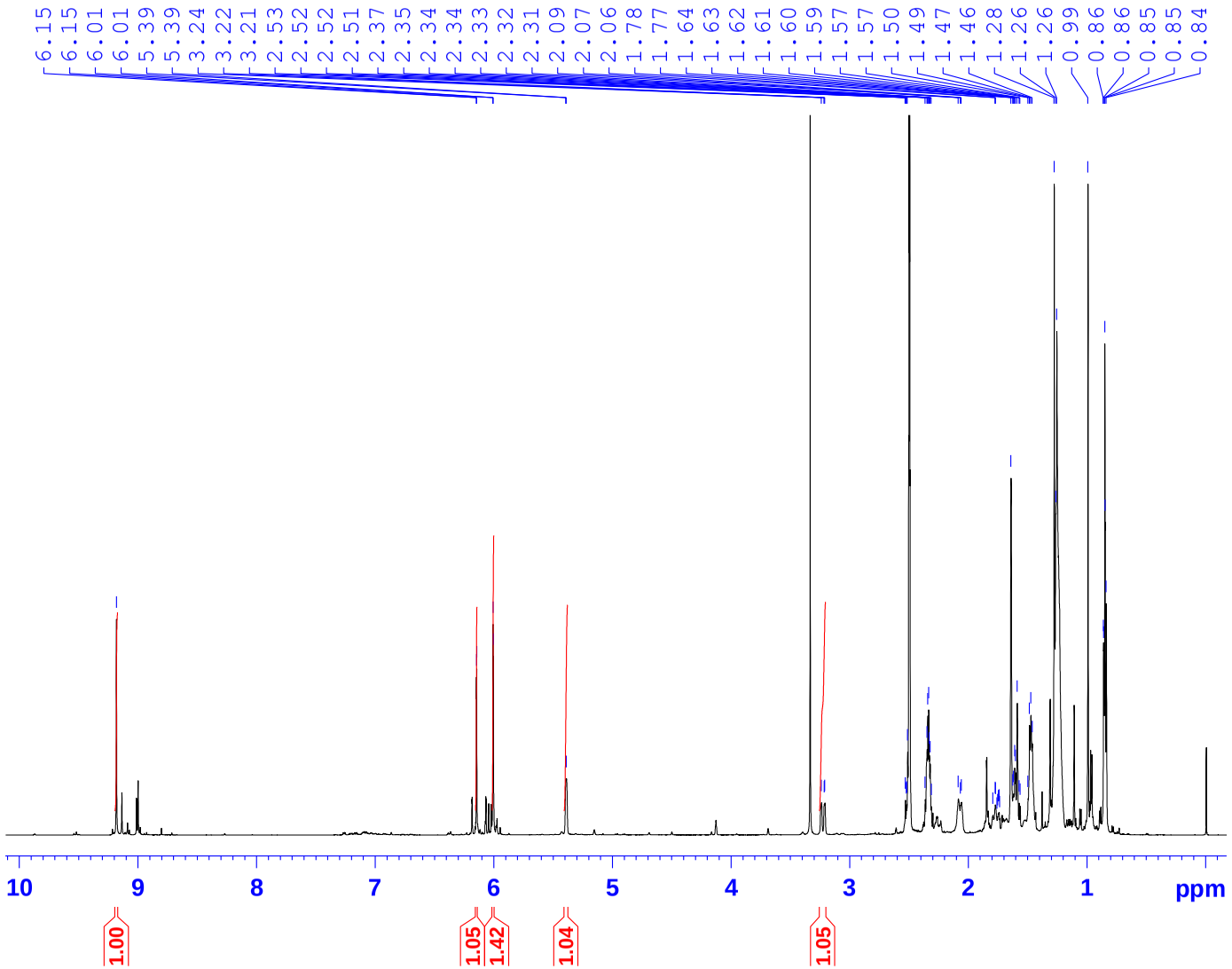
University
*of Ljubljana*

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: | **3227-22** |
| Received date: | April 4, 2023 |
| Our notebook code: | NFL-3227-22 |
| NMR sample preparation: | 21 mg dissolved in 0.7 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-$^1$H NOESY, $^{13}$C DEPT-135, $^{13}$C DEPT-90 |
| Proposed structure with formula, exact mass, molecular weight: |  Chemical Formula: $C_{23}H_{34}O_2$<br>Exact Mass: 342,2559<br>Molecular Weight: 342,5230 |
| Chemical name: | 3-Heptyl-6a,7,10,10a-tetrahydro-6,6,9-trimethyl-6*H*-dibenzo[*b*,*d*]pyran-1-ol |
| Comments: | - Structure elucidation based on 1D and 2D NMR spectra and HRMS.<br>- cca. 70% purity of a sample based on $^1$H NMR spectrum. Contains hexane and traces of structurally similar cannabinoids. |
| 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 19, 2023 |

NFL-3227-22
1H




Current Data Parameters

| | |
|---|---|
| NAME | NFL-3227-22 |
| EXPNO | 1 |
| PROCNO | 1 |

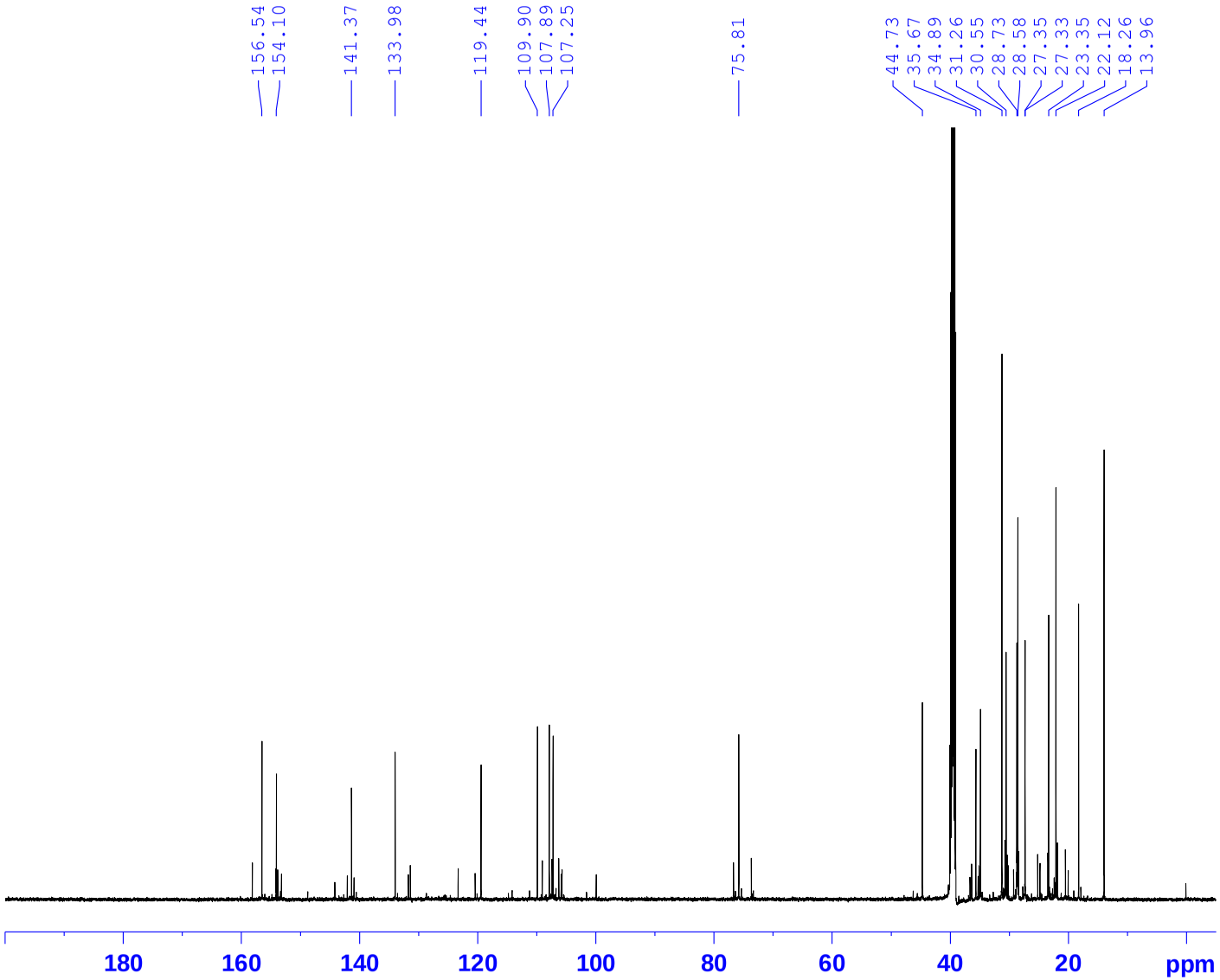
F2 - Acquisition Parameters

| | | |
|---|---|---|
| Date_ | 20230409 | |
| Time | 14.00 | 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 | 296.2 | 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 | 600.1300049 | MHz |
| WDW | EM | |
| SSB | 0 | |
| LB | 0.30 | Hz |
| GB | 0 | |
| PC | 1.00 | |

NFL-3227-22
13C {1H}




Current Data Parameters

| | |
|---|---|
| NAME | NFL-3227-22 |
| EXPNO | 6 |
| PROCNO | 1 |

F2 - Acquisition Parameters

| | |
|---|---|
| Date_ | 20230410 |
| Time | 8.08 h |
| INSTRUM | AV600 NEO |
| PROBHD | Z176567_0002 ( |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | DMSO |
| NS | 10240 |
| 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 | 2.00000000 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 | 150.9028790 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 1.00 Hz |
| GB | 0 |
| PC | 1.40 |