



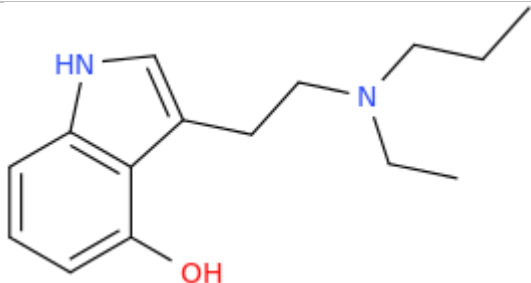
ANALYTICAL REPORT

4-HO-EPT (C₁₅H₂₂N₂O)

3-{2-[ethyl(propyl)amino]ethyl}-1H-indol-4-ol

Remark – other NPS detected: **none**

Sample ID:	2026-18
Sample description:	powder
Sample type:	test purchase /NFL- purchasing
Date of entry (DD/MM/YYYY) into NFL database:	14/01/2020
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-[ethyl(propyl)amino]ethyl}-1H-indol-4-ol
Other names	
Formula (per base form)	C ₁₅ H ₂₂ N ₂ O
M _w (g/mol)	246,35
Salt form/anions detected	fumarate
StdInChIKey (per base form)	JQLEPKHBXEAHR-UHFFFAOYSA-N
Other NPS detected	none
Additional info (purity..)	>95% pure based on ¹ H 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 °C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 µm. 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 7.1 min, then heating at 50 °C/min up to 325 °C and finally 6.1 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 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 condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)

GC-method: Injection volume 1 µl 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 µl

Supporting information

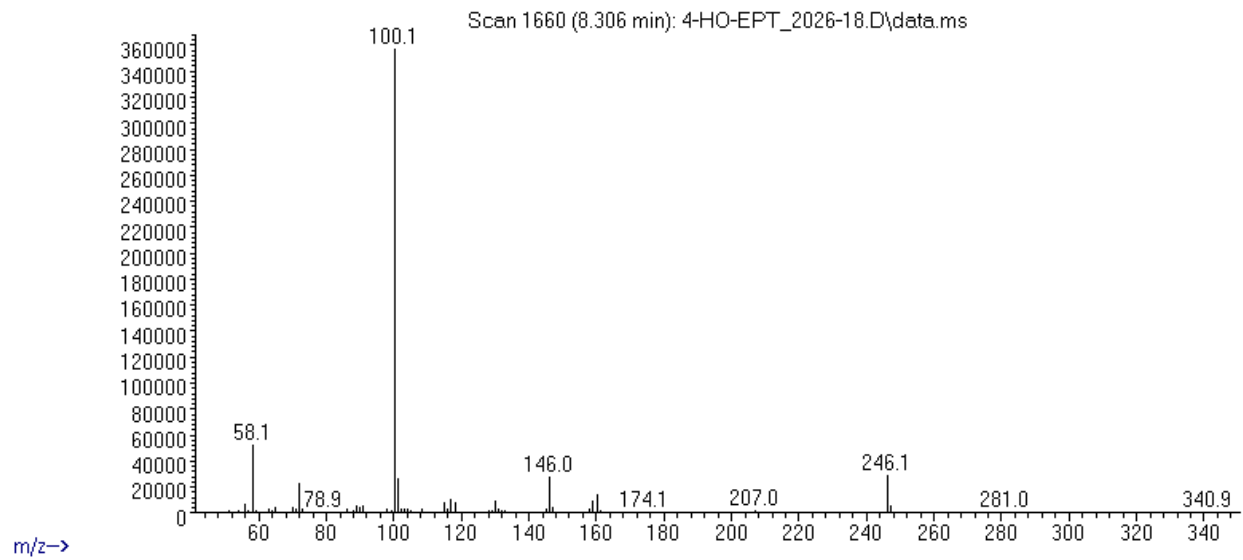
Solubility in	result/remark
CH ₂ Cl ₂	partially
MeOH	partially
H ₂ O	not soluble

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 8,31 BP(1): 100; BP(2): 58,BP(3) :246,
HPLC-TOF	+	Exact mass (theoretical): 246,1732; measured value Δppm:-1,04; formula:C15H22N2O
FTIR-ATR	+	direct measurement (sample as received)
FTIR (solid phase) always as base form	+	
IC (anions)	-	
NMR (in FKKT)	+	
validation		
other		

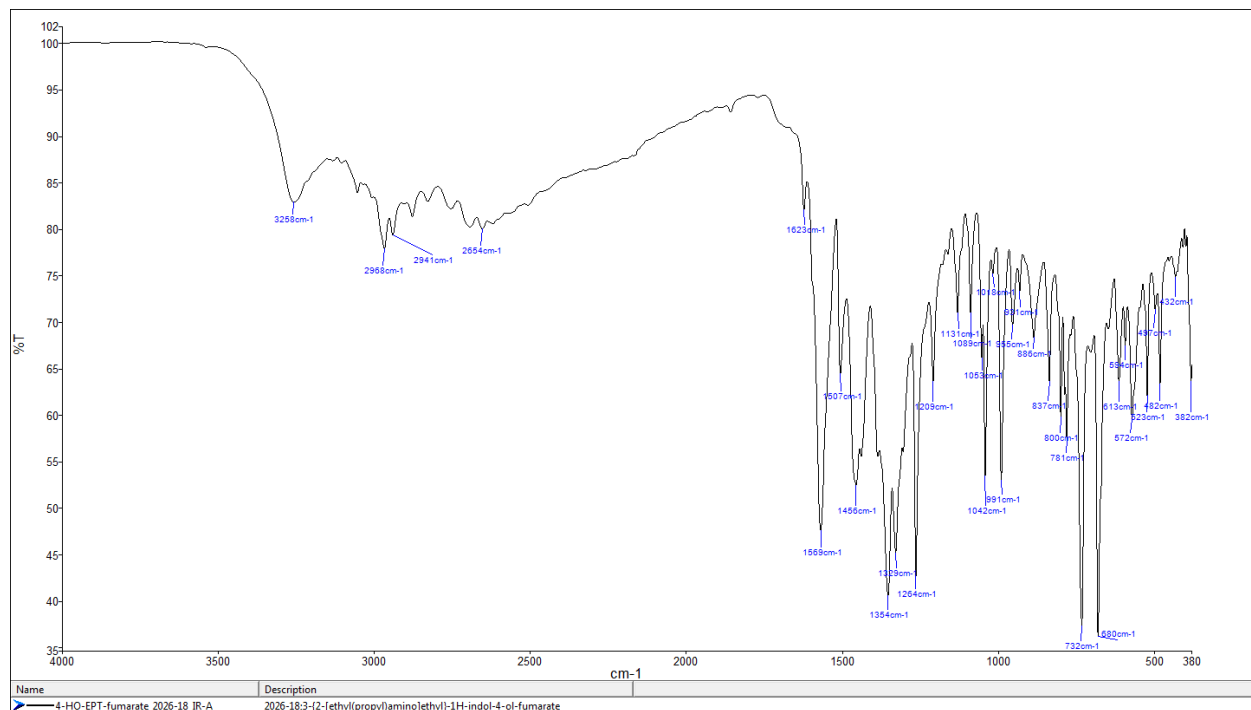
ANALYTICAL RESULTS

MS (EI)

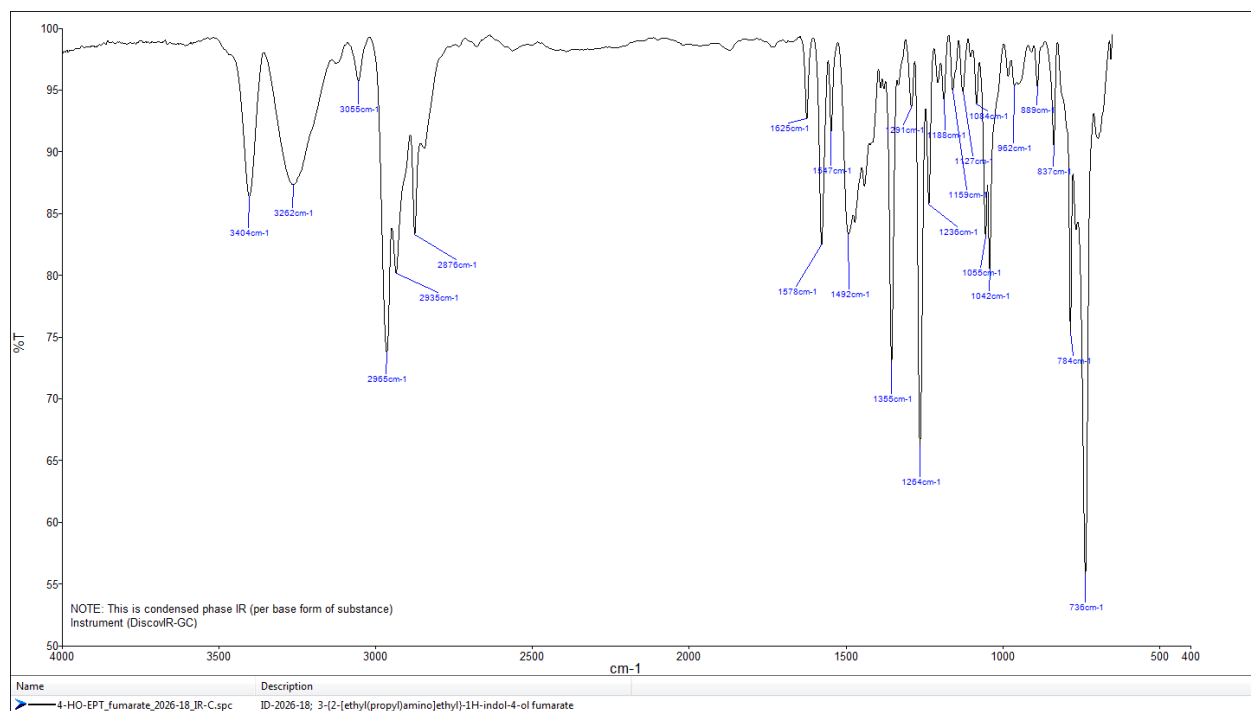
Abundance



FTIR-ATR - direct measurement (sample as received)



IR (solid phase – after chromatographic separation)



TOF REPORT

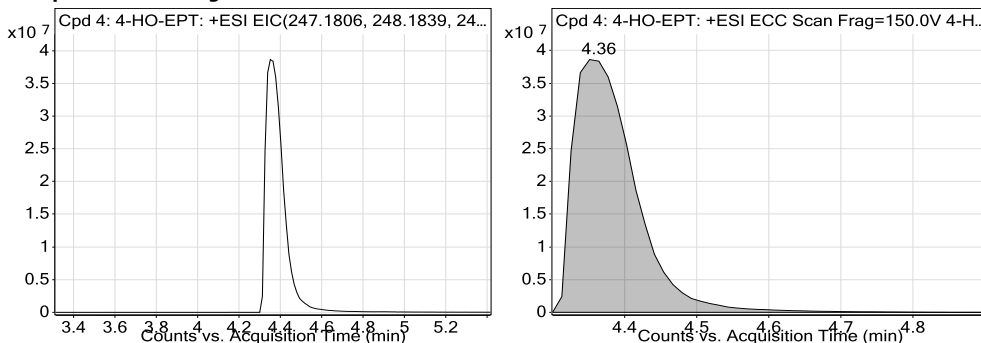
Data File	4-HO-EPT_2026_18.d	Sample Name	ID 2026-18
Sample Type	Sample	Position	P2-F6
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	general-19_10_2018-XDB-C18-ESI+.m	Acquired Time	11/20/2018 12:39:58 PM
IRM Calibration Status	Success	DA Method	a-Drugs_NFL.m
Comment	MeOH		

Compound Table

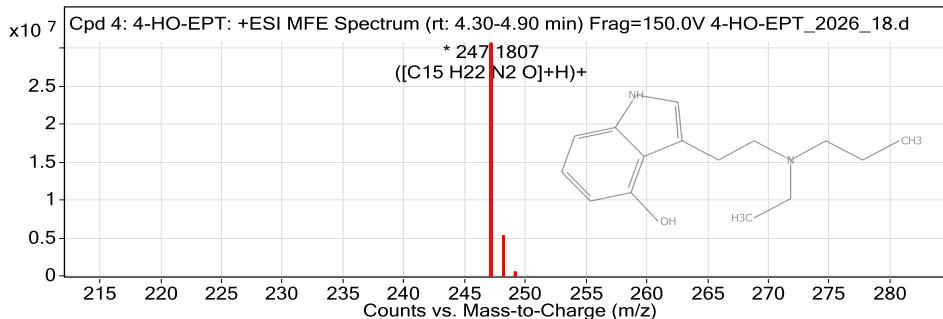
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 4: 4-HO-EPT	4-HO-EPT	C15 H22 N2 O	4.36	246.1735

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
4-HO-EPT	247.1807	4.36	246.1735	4.36	C15 H22 N2 O	246.1732	-1.04

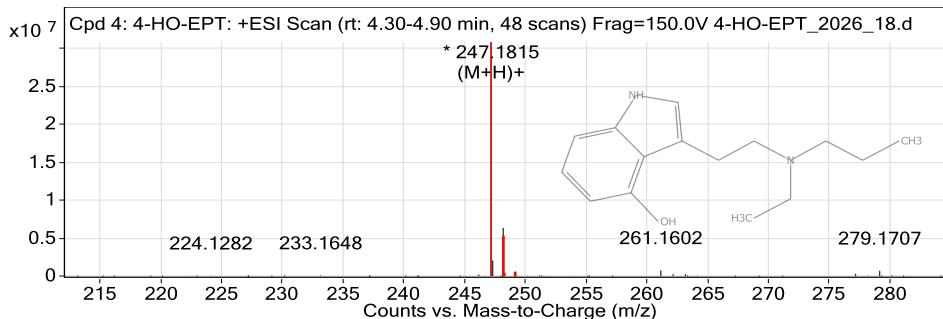
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

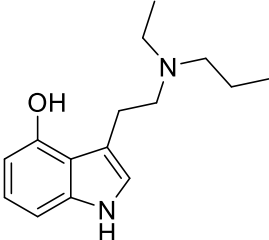
Obs. m/z	Charge	Abund	Formula	Ion/Isotope
247.1807	1	30866112	C15 H22 N2 O	(M+H)+
248.184	1	5086825.91	C15 H22 N2 O	(M+H)+
249.1874	1	421487.97	C15 H22 N2 O	(M+H)+
250.1899	1	27470.79	C15 H22 N2 O	(M+H)+

--- End Of Report ---

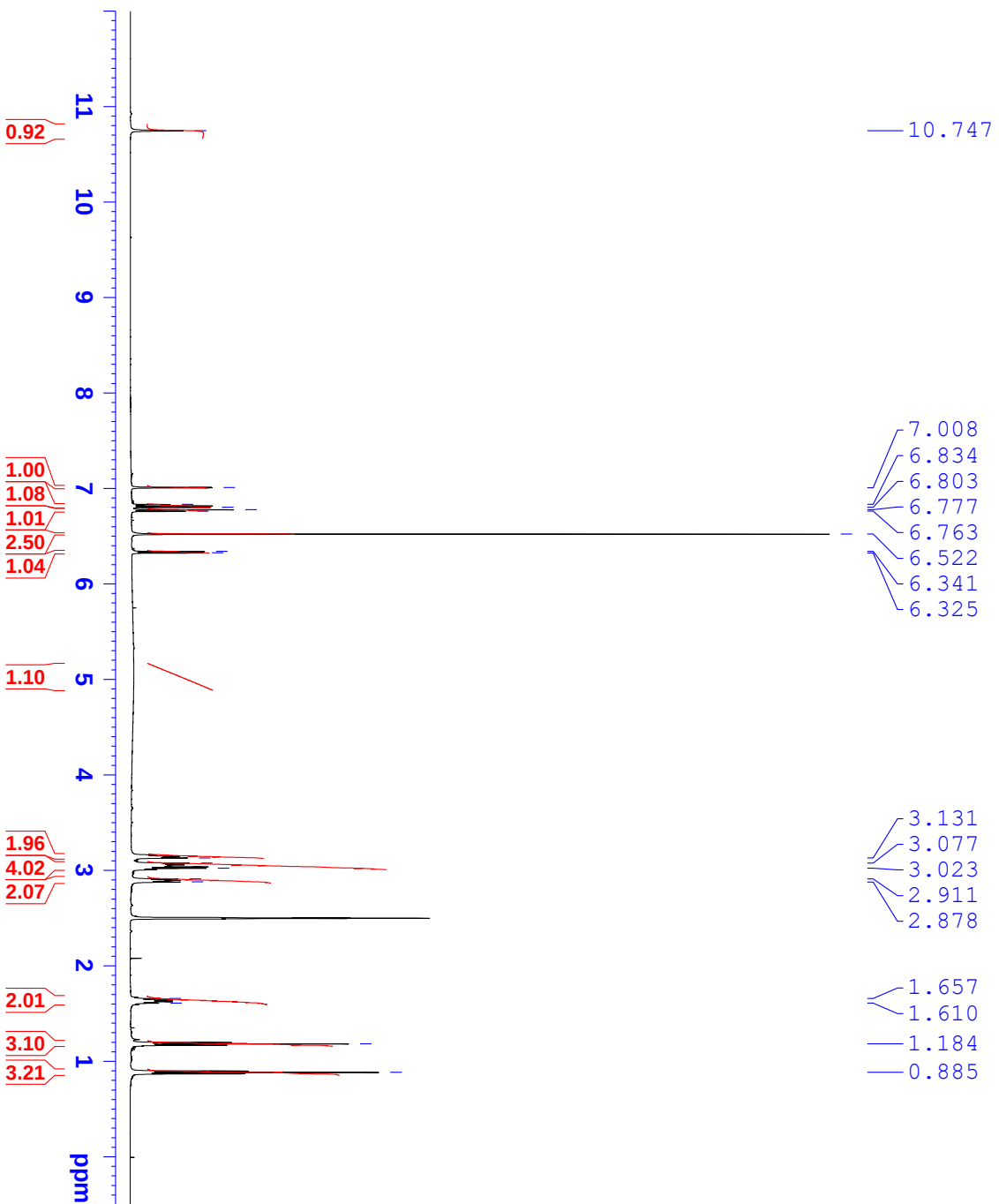
University
of Ljubljana
Faculty of Chemistry
and Chemical Technology



R E P O R T

Contract No.	C1714-19-460155 (Republic of Slovenia, Ministry of the Interior, POLICE)
Sample ID:	2026-18
Received date:	November 27, 2019
Our notebook code:	NFL-2026-18
NMR sample preparation:	20.7 mg dissolved in 0.7 mL DMSO- <i>d</i> ₆
NMR experiments:	¹ H, ¹³ C, ¹ H- ¹ H <i>gs</i> -COSY, ¹ H- ¹³ C <i>gs</i> -HSQC, ¹ H- ¹³ C <i>gs</i> -HMBC, ¹ H- ¹⁵ N <i>gs</i> -HMBC
Proposed structure with formula, exact mass, molecular weight:	 Chemical Formula: C₁₅H₂₂N₂O Exact Mass: 246,1732 Molecular Weight: 246,3540
Chemical name:	3-(2-(ethyl(propyl)amino)ethyl)-1 <i>H</i> -indol-4-ol
Comments:	- Structure elucidation based on 1D and 2D NMR spectra and HRMS. - The sample consists of herein identified compound and presumably fumarate in molar ratio 1 : 1.25, based on ¹H NMR spectrum. - >95% purity of a sample based on ¹H 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:	December 5, 2019

NFL-2026-18
¹H



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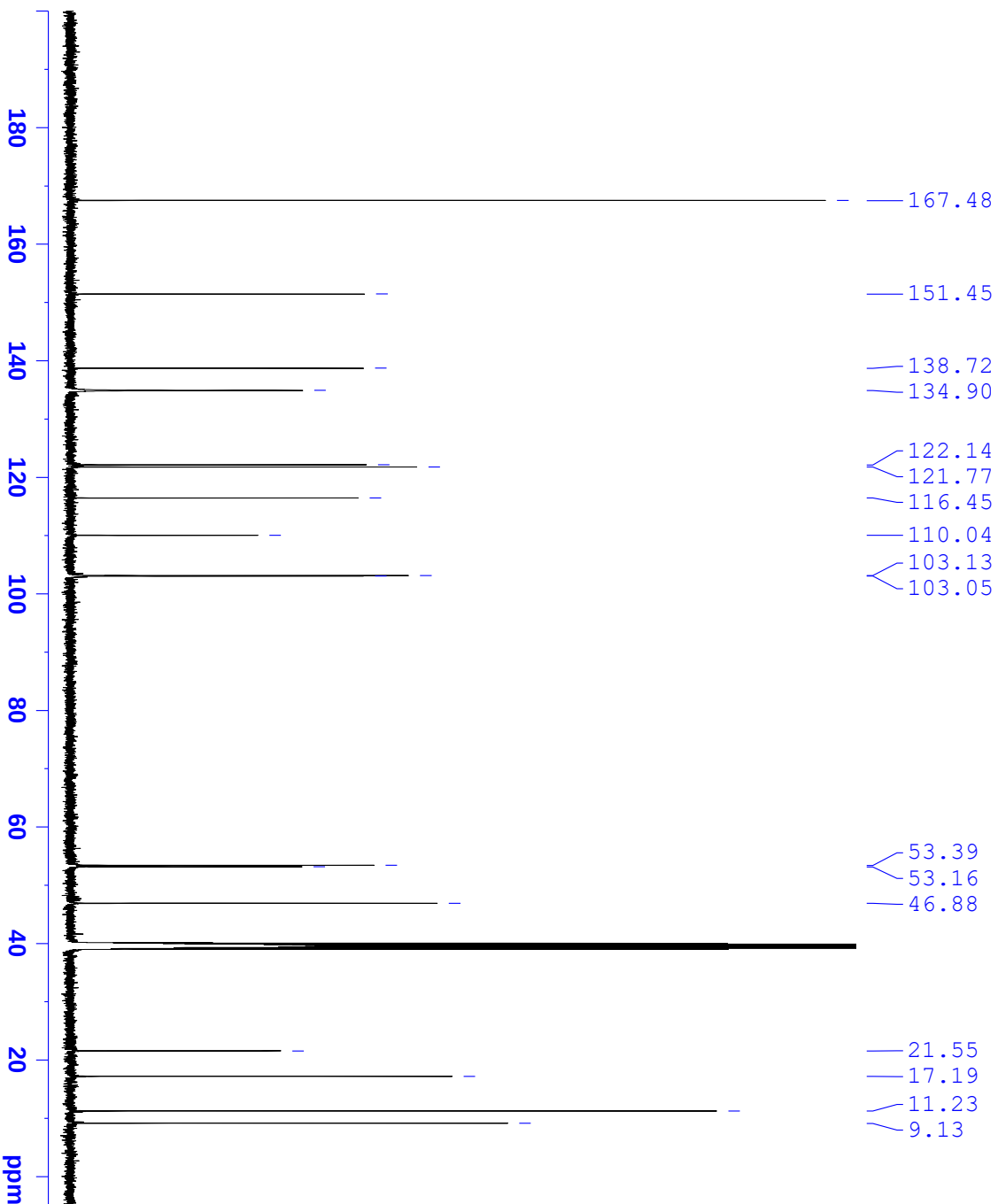
Current Data Parameters
NAME                NFL-2026-18
EXPNO                1
PROCNO              1

F2 - Acquisition Parameters
Date_                20191127
Time_                22.22
INSTRUM              spect
PROBHD               5 mm PABBO BB-
PULPROG              zg30
TD                   65536
SOLVENT              DMSO
NS                   16
DS                   2
SWH                  10000.000 Hz
FIDRES               0.152588 Hz
AQ                   3.2767999 sec
RG                   71.8
DW                   50.000 usec
DE                   6.50 usec
TE                   296.0 K
D1                   1.00000000 sec
TD0                  1

===== CHANNEL f1 =====
SFO1                 500.1330885 MHz
NUC1                 1H
P1                   8.70 usec
PLW1                 26.00000000 W

F2 - Processing parameters
SI                   65536
SF                   500.1300042 MHz
WDW                  EM
SSB                  0
LB                   0.30 Hz
GB                   0
PC                   1.00
  
```

NFL-2026-18
13C



Current Data Parameters
NAME NFL-2026-18
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191128
Time_ 0.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 8.70 usec
PLW1 122.00000000 W

===== CHANNEL f2 =====
SFO2 500.132005 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 80.00 usec
PLW2 26.00000000 W
PLW12 0.30046001 W
PLW13 0.15113001 W

F2 - Processing parameters
SI 32768
SF 125.7578416 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40