NACIONALNI FORENZIČNI LABORATORIJ
NATIONAL FORENSIC LABORATORY
Vodovodna 95, 1000 LJUBLJANA, SLOVENIA

T: +386 (0)1 428 44 93
E: nfl@policija.si
www.policija.si

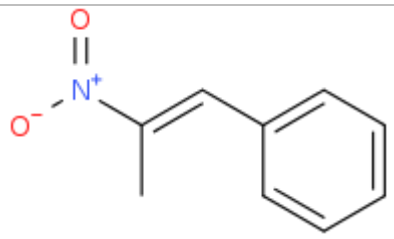
ANALYTICAL REPORT

P2NP (C9H9NO2)

2-nitroprop-1-en-1-yl benzene

Remark – other NPS detected: none

Sample ID:	1721-16
Sample description:	crystalinic
Sample type:	seized /MB
Date of sample receipt (M/D/Y):	9/30/2016
Date of entry (M/D/Y) into NFL database:	10/24/2017
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-nitroprop-1-en-1-yl benzene
Other names	NSC 2014; P2NP; phenyl-2-nitropropene; 1-phenyl-2-nitropropene; methylnitrostyrene; trans-β-Methyl-β-nitrostyrene; β-Methyl-β-nitrostyrene; (2-Nitroprop-1-en-1-yl)benzene; Benzene, (2-nitro-1-propenyl)-; 2-Nitro-1-phenylpropene
Formula (per base form)	C9H9NO2
M_w (g/mol)	163,18
Salt form/anions detected	base
StdInChIKey (per base form)	WGSVFWFSJDAYBM-UHFFFAOYSA-N
Other NPS detected	none
Additional info (purity..)	impurity benzaldehyde detected by GC-MS

[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 ml 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 7.1 min, then heating at 50 ^{0}C/min up to 325 ^{0}C and finally 6.1 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 condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)
GC-method: Injection volume 1 ml 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 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

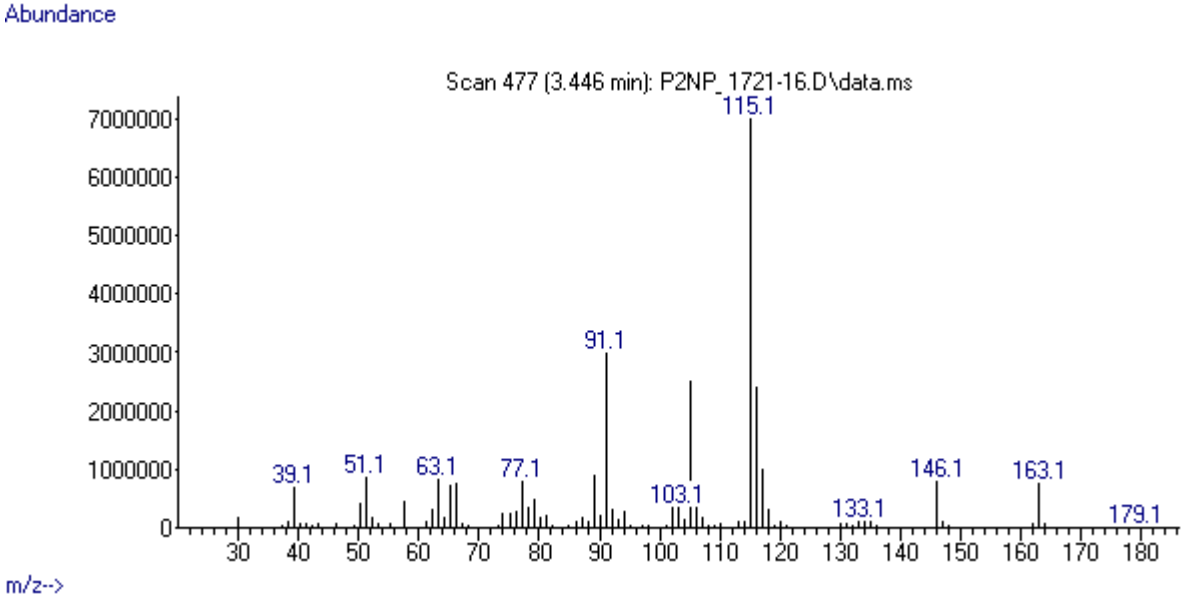
Supporting information

Solubility in	result/remark
CH_2Cl_2	soluble
MeOH	soluble
H_2O	

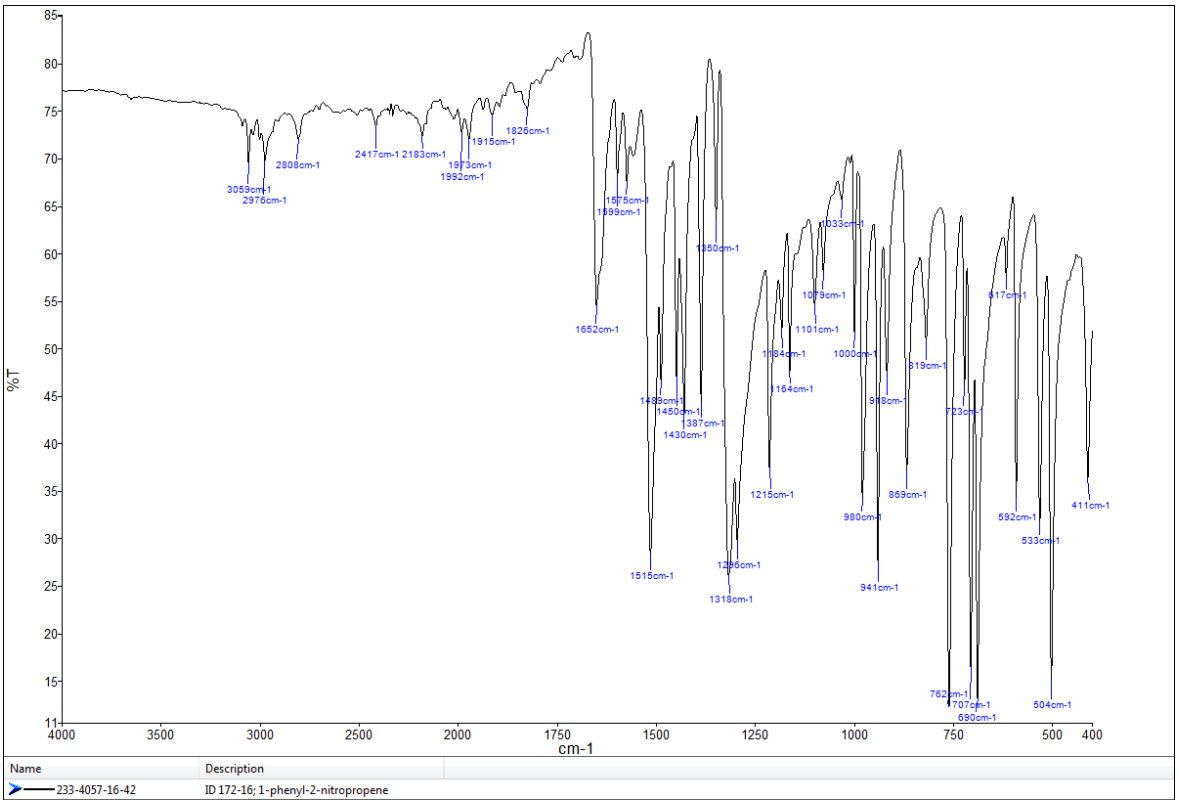
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 3,45 BP(1): 115; BP(2): 91,BP(3) :105,
HPLC-TOF	-	Exact mass (theoretical): na; measured value Δppm:na; formula:C9H9NO2
FTIR-ATR	+	direct measurement (sample as received)
FTIR (condensed phase) always as base form	+	
IC (anions)		
NMR (in FKKT)	+	
validation		see NMR report
other		

ANALYTICAL RESULTS

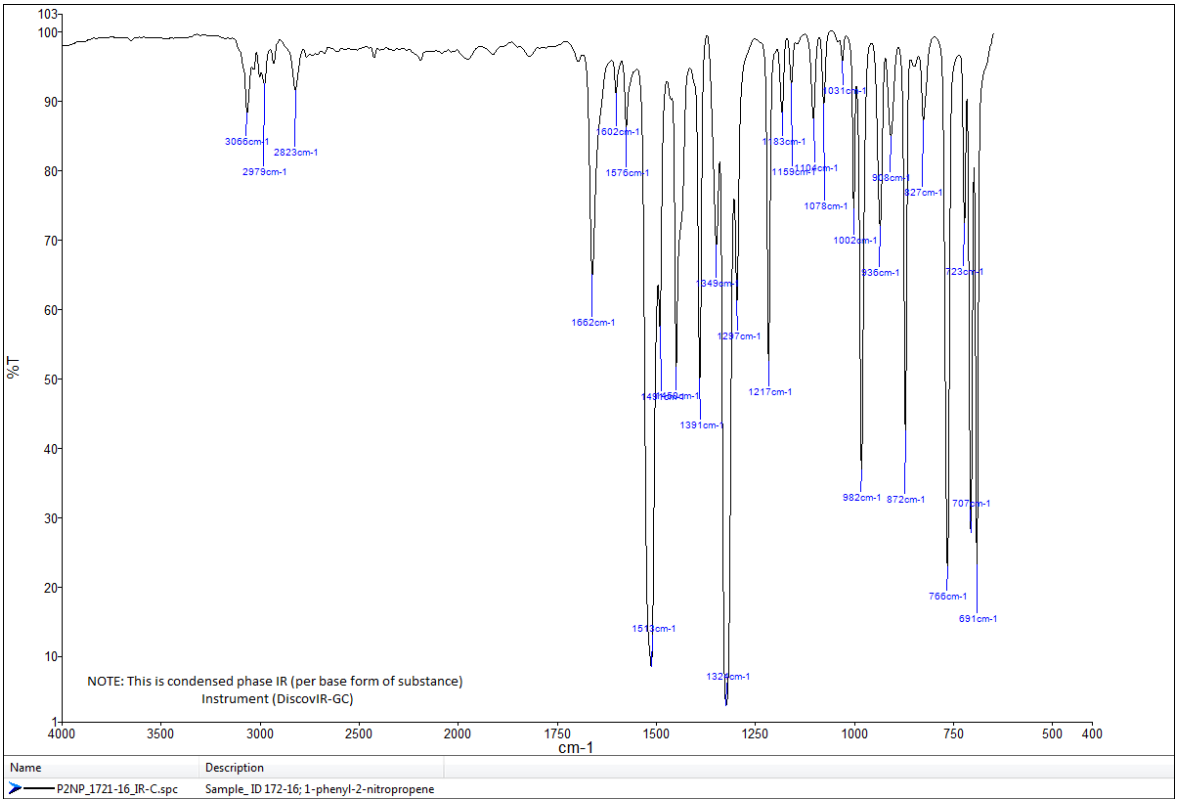
MS (EI)



FTIR-ATR - direct measurement (sample as received)



IR (condensed phase – after chromatographic separation)

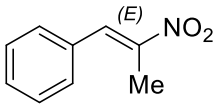


University
of Ljubljana

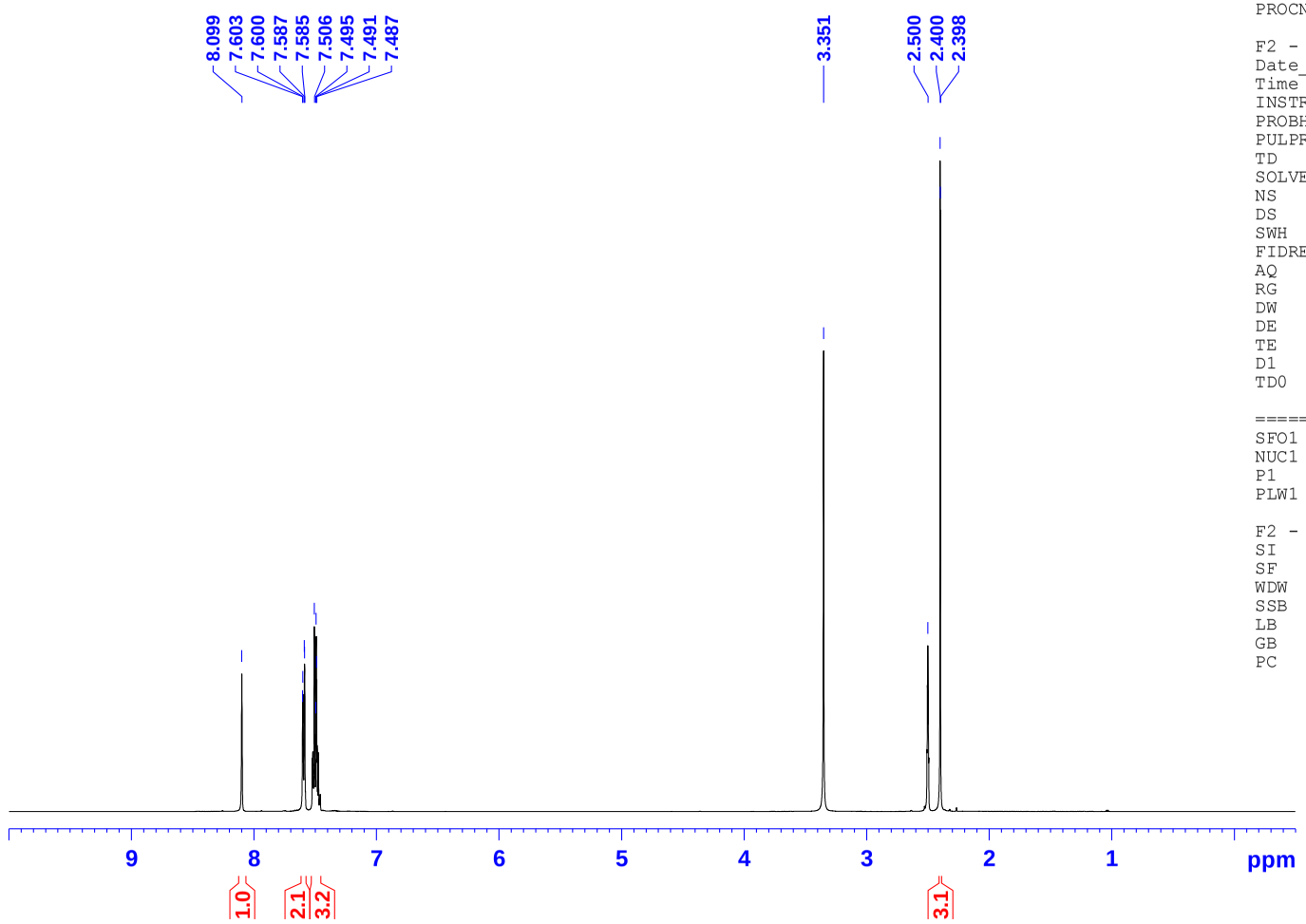
Faculty *of Chemistry and Chemical Technology*

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

R E P O R T

Contract No.	C1714-17-460078 (Republic of Slovenia, Ministry of the Interior, POLICE)
Sample ID:	**1721-16**
Received date:	October 10, 2017
Our notebook code:	P-1721-16
NMR sample preparation:	12 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–^{15}N *gs*-HMBC
Proposed structure with atom numbering scheme, formula, exact mass, molecular weight:	 Chemical Formula: $C_9H_9NO_2$ Exact Mass: 163,0633 Molecular Weight: 163,1760
Chemical name:	(*E*)-(2-Nitroprop-1-en-1-yl)benzene
Comments:	- Structure elucidation based on 1D and 2D NMR spectra. - The result is consistent with the suggested chemical formula. - Spectroscopic data are in agreement with the literature report (A. Fryszkowska, K. Fisher, J. M. Gardiner, G. M. Stephens, *J. Org. Chem.* **2008**, *73*, 4295–4298).
Supporting information:	Copies of ^{1}H and ^{13}C NMR spectra
Authors:	Martin Gazvoda, Marko Krivec, Janez Košmrlj
Date of report:	October 21, 2017

P-1721-16

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Current Data Parameters
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PROCNO                1

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PULPROG            zg30
TD                65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2768500 sec
RG                 80.6
DW                50.000 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                   1

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NUC1                 1H
P1                 8.70 usec
PLW1        26.00000000 W

F2 - Processing parameters
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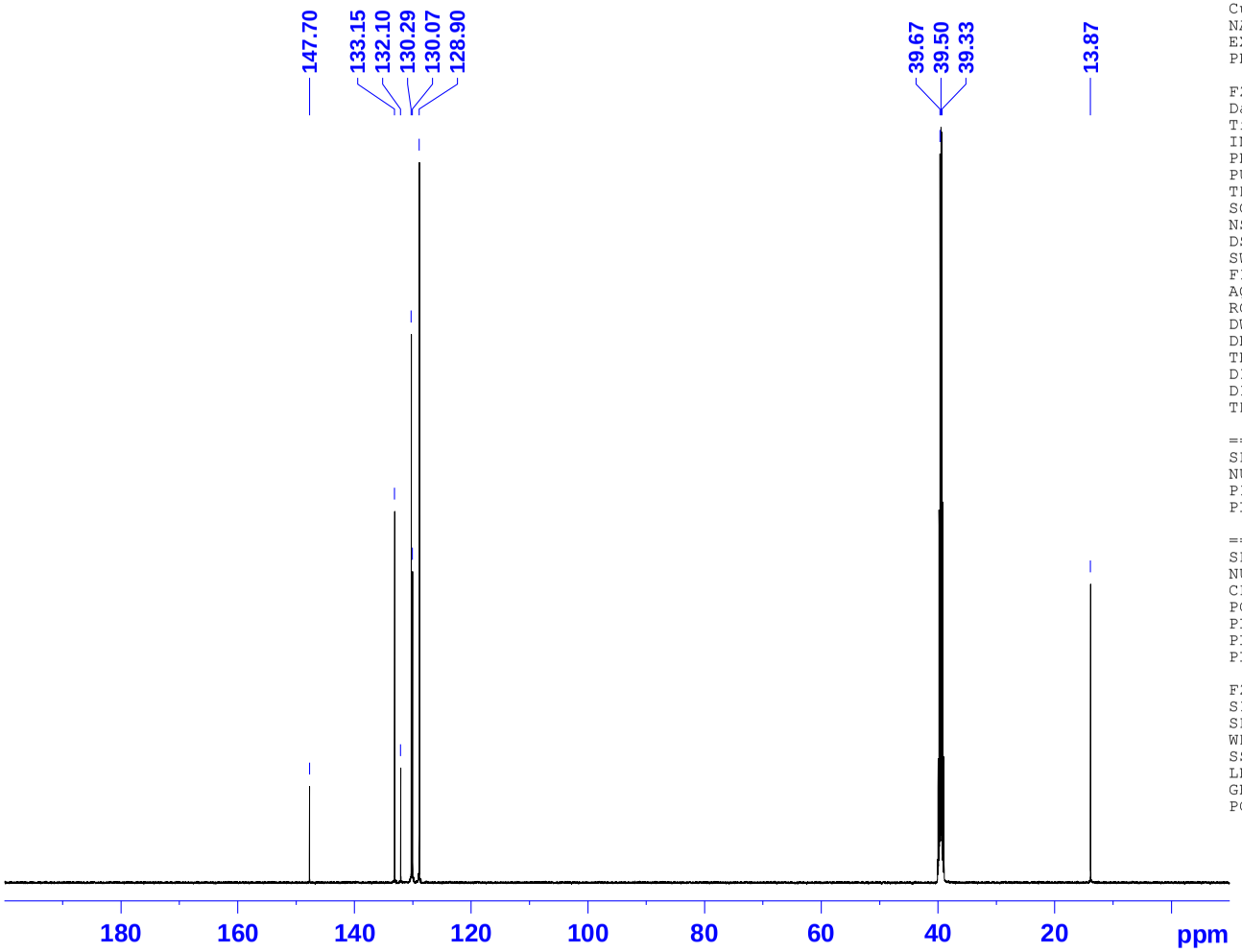
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

P-1721-16

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Current Data Parameters
NAME                  P-1721-16
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
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Time                       5.48
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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                         1030
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                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2                26.00000000 W
PLW12                0.30046001 W
PLW13                0.15113001 W

F2 - Processing parameters
SI                        32768
SF                  125.7577885 MHz
WDW                          EM
SSB               0
LB                        1.00 Hz
GB                0
PC                        1.40
```