## ANALYTICAL REPORT

**P2NP (C9H9NO2)**

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

**Remark** – other NPS detected: **none**

<table>
<thead>
<tr>
<th><strong>Sample ID</strong></th>
<th>1721-16</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Sample description</strong></td>
<td>crystalinic</td>
</tr>
<tr>
<td><strong>Sample type</strong></td>
<td>seized /MB</td>
</tr>
<tr>
<td><strong>Date of sample receipt (M/D/Y)</strong></td>
<td>9/30/2016</td>
</tr>
<tr>
<td><strong>Date of entry (M/D/Y) into NFL database</strong></td>
<td>10/24/2017</td>
</tr>
</tbody>
</table>

**Substance identified - structure**

![Structure of 2-nitroprop-1-en-1-yl benzene](image)

- **Systematic name**: 2-nitroprop-1-en-1-yl benzene
- **Other names**: NSC 2014; P2NP; phenyl-2-nitropropene; 1-phenyl-2-nitropropene; methyl nitrostyrene; 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
- **Mw (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

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1 Created by OPSIN free tool: [http://opsin.ch.cam.ac.uk/](http://opsin.ch.cam.ac.uk/)  DOI: 10.1021/ci100384d
Report updates

<table>
<thead>
<tr>
<th>date</th>
<th>comments (explanation)</th>
</tr>
</thead>
<tbody>
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<td></td>
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</tbody>
</table>

**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 °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 ml 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 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

<table>
<thead>
<tr>
<th>Solubility in</th>
<th>result/remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH$_2$Cl$_2$</td>
<td>soluble</td>
</tr>
<tr>
<td>MeOH</td>
<td>soluble</td>
</tr>
<tr>
<td>H$_2$O</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Analytical technique:</th>
<th>applied</th>
<th>remarks</th>
</tr>
</thead>
</table>
| 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: C$_9$H$_9$NO$_2$ |
| 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)

Abundance

Scan 477 (3.446 min): P2NP_1721-16_D\data.ms

m/z→

ID 1721-16
FTIR-ATR - direct measurement (sample as received)

IR (condensed phase – after chromatographic separation)

NOTE: This is condensed phase IR (per base form of substance)
Instrument (Discovery GC)
## REPORT

<table>
<thead>
<tr>
<th>Contract No.</th>
<th>C1714-17-460078 (Republic of Slovenia, Ministry of the Interior, POLICE)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample ID:</td>
<td>1721-16</td>
</tr>
<tr>
<td>Received date:</td>
<td>October 10, 2017</td>
</tr>
<tr>
<td>Our notebook code:</td>
<td>P-1721-16</td>
</tr>
<tr>
<td>NMR sample preparation:</td>
<td>12 mg dissolved in 0.7 mL DMSO-d$_6$</td>
</tr>
<tr>
<td>NMR experiments:</td>
<td>$^1$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</td>
</tr>
</tbody>
</table>
| Proposed structure with atom numbering scheme, formula, exact mass, molecular weight: | ![Chemical Structure](image)  
\[\text{Chemical Formula: } C_9H_9NO_2\]  
\[\text{Exact Mass: } 163.0633\]  
\[\text{Molecular Weight: } 163.1760\] |
| 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.  
| Supporting information: | Copies of $^1$H and $^{13}$C NMR spectra                               |
| Authors: | Martin Gazvoda, Marko Krivec, Janez Košmrlj                            |
| Date of report: | October 21, 2017                                                      |
Current Data Parameters

NAME          p-1721-16
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20171013
Time               3.45
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            3.2768500 sec
RG                 80.6
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          500.1300041 MHz
WDW                  EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00

P-1721-16

\[\text{Diagram with spectral data}\]