

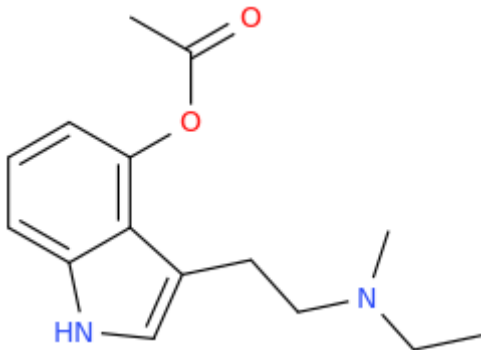
## ANALYTICAL REPORT

4-AcO-MET (C<sub>15</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub>)

## 3-{2-[ethyl(methyl)amino]ethyl}-1H-indol-4-yl acetate

Remark – other NPS detected:

|   |   |
|---|---|
| Sample ID:                                      | 2226-20   |
| Sample description:                             | powder  |
| Sample type:                                    | test purchase /ISF projekt (NFL-SI)   |
| Date of entry (DD/MM/YYYY) into NFL database:   | 10/02/2021  |
| Report updates (if any) will be published here: | <a href="http://www.policija.si/apps/nfl_response_web/seznam.php">http://www.policija.si/apps/nfl_response_web/seznam.php</a> |

|   |   |
|---|---|
| Substance identified - structure <sup>1</sup> (base form) |  |
| Systematic name   | 3-{2-[ethyl(methyl)amino]ethyl}-1H-indol-4-yl acetate                               |
| Other names   | 4-Acetoxy-N-ethyl-N-methyltryptamine; 4-Acetoxy MET                                 |
| Formula (per base form)                                   | C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>                       |
| M <sub>w</sub> (g/mol)                                    | 260,34  |
| Salt form/anions detected                                 | fumarate  |
| StdInChIKey (per base form)                               | OMDKHOOGGJRLX-UHFFFAOYSA-N  |
| Other NPS detected  |   |
| Additional info (purity..)                                | minor impurities observed by GC-MS  |

<sup>1</sup> 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 (N<sub>2</sub>) 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<sup>-1</sup>; resolution 4cm<sup>-1</sup>

**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<sup>-1</sup>.

**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

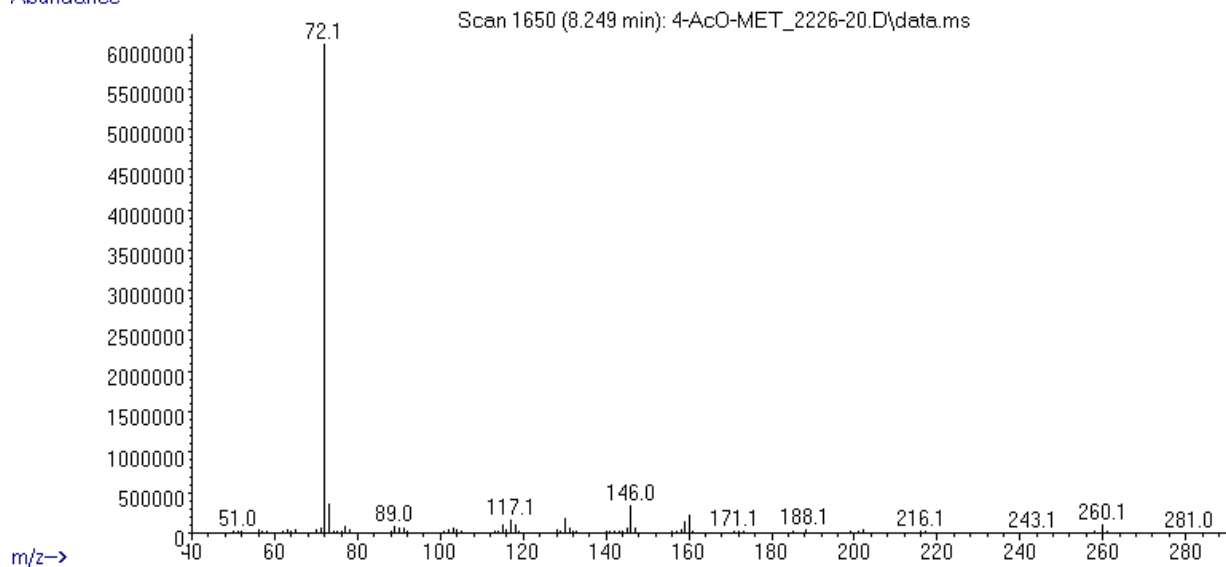
| Solubility in                   | result/remark |
|---------------------------------|---------------|
| CH <sub>2</sub> Cl <sub>2</sub> | low (bad)     |
| MeOH                            | soluble       |
| H <sub>2</sub> O                | partially     |

| Analytical technique:                  | applied | remarks  |
|--|---------|--|
| GC-MS (EI ionization)                  | +       | NFL GC-RT (min): 8,25<br>BP(1): 72; BP(2): 73,BP(3) :146,  |
| HPLC-TOF                               | +       | Exact mass (theoretical): 260,1525;<br>measured value Δppm:-1,91;<br>formula:C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> |
| FTIR-ATR                               | +       | direct measurement (sample as received)  |
| FTIR (solid phase) always as base form | +       |  |
| IC (anions)                            | +       |  |
| NMR (in FKKT)                          |         |  |
| validation                             |         |  |
| other                                  |         |  |

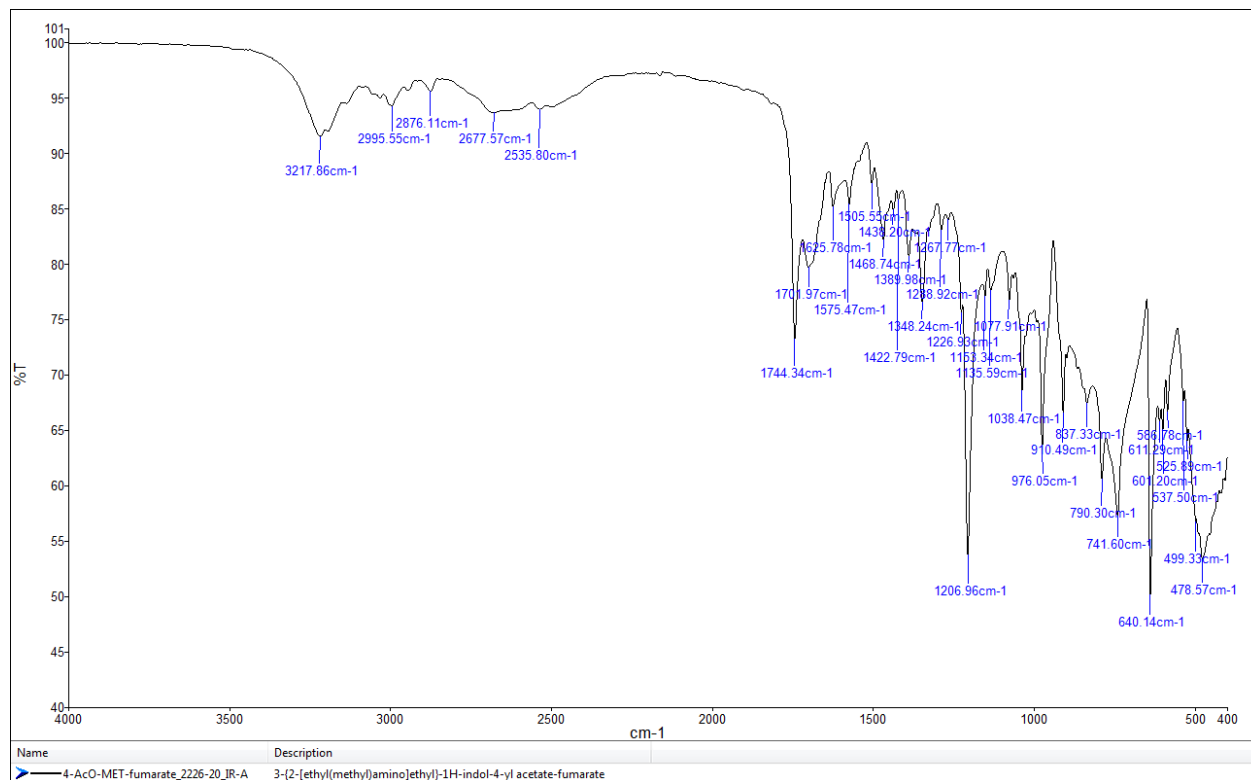
# ANALYTICAL RESULTS

MS (EI)

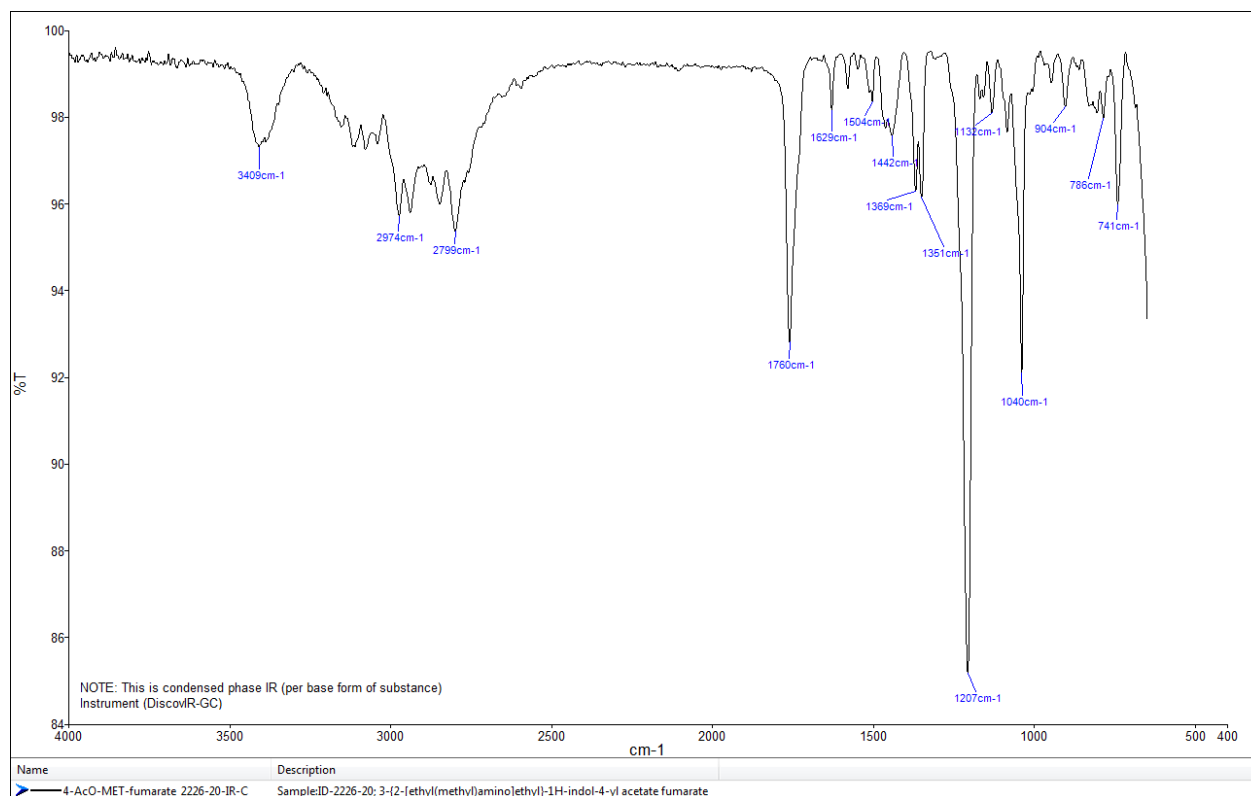
Abundance



## FTIR-ATR - direct measurement (sample as received)



## IR (solid phase – after chromatographic separation)



# TOF REPORT

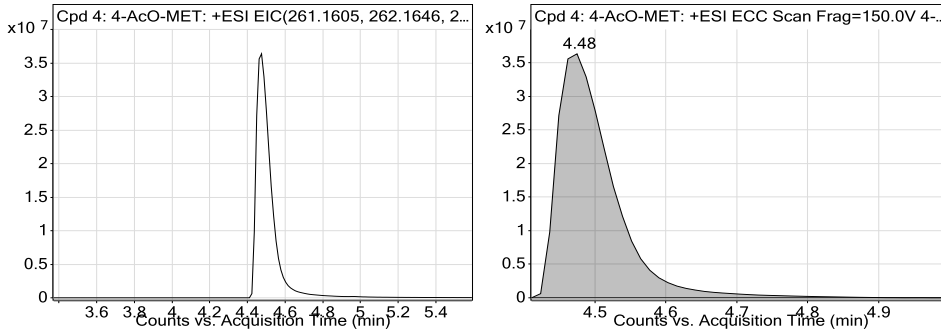
|                               |                                   |                      |                       |
|-------------------------------|-----------------------------------|----------------------|-----------------------|
| <b>Data File</b>              | 4-AcO-MET_2226_20.d               | <b>Sample Name</b>   | ID-2226-20            |
| <b>Sample Type</b>            | Sample                            | <b>Position</b>      | P1-A9                 |
| <b>Instrument Name</b>        | 6230B TOF LC-MS                   | <b>User Name</b>     | TG                    |
| <b>Acq Method</b>             | general-15_01_2020-XDB-C18-ESI+.m | <b>Acquired Time</b> | 12/4/2020 10:30:40 AM |
| <b>IRM Calibration Status</b> | Success                           | <b>DA Method</b>     | a-Drugs_NFL.m         |
| <b>Comment</b>                | MeOH                              |                      |                       |

## Compound Table

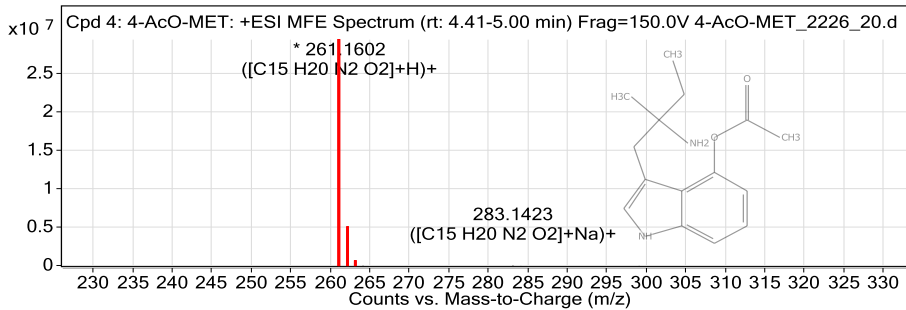
| Label            | Compound Name | MFG Formula   | Obs. RT | Obs. Mass |
|------------------|---------------|---------------|---------|-----------|
| Cpd 4: 4-AcO-MET | 4-AcO-MET     | C15 H20 N2 O2 | 4.48    | 260.153   |

| Name      | Obs. m/z | Obs. RT | Obs. Mass | DB RT | DB Formula    | DB Mass  | DB Mass Error (ppm) |
|-----------|----------|---------|-----------|-------|---------------|----------|---------------------|
| 4-AcO-MET | 261.1602 | 4.48    | 260.153   | 4.42  | C15 H20 N2 O2 | 260.1525 | -1.91               |

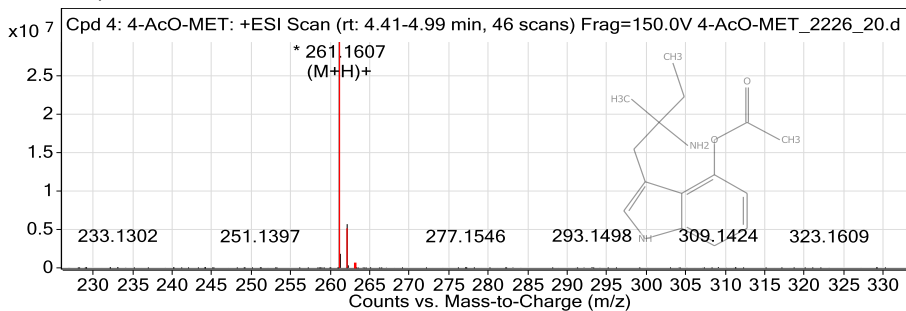
## Compound Chromatograms



## MFE MS Zoomed Spectrum



## MS Zoomed Spectrum



## MS Spectrum Peak List

| Obs. m/z | Charge | Abund     | Formula       | Ion/Isotope |
|----------|--------|-----------|---------------|-------------|
| 261.1602 | 1      | 29351782  | C15 H20 N2 O2 | (M+H)+      |
| 262.1636 | 1      | 5100245.3 | C15 H20 N2 O2 | (M+H)+      |
| 263.1665 | 1      | 493388.61 | C15 H20 N2 O2 | (M+H)+      |
| 264.1688 | 1      | 40121.35  | C15 H20 N2 O2 | (M+H)+      |
| 283.1423 | 1      | 54412.93  | C15 H20 N2 O2 | (M+Na)+     |
| 284.1455 | 1      | 9947.51   | C15 H20 N2 O2 | (M+Na)+     |
| 299.1162 | 1      | 14628.13  | C15 H20 N2 O2 | (M+K)+      |

--- End Of Report ---

### Peak Integration Report

|                   |                     |                  |        |
|-------------------|---------------------|------------------|--------|
| Sample Name:      | 2226_IC             | Inj. Vol.:       | 25,00  |
| Injection Type:   | Unknown             | Dilution Factor: | 1,0000 |
| Program:          | ANIONI              | Operator:        | Admin  |
| Inj. Date / Time: | 04-Dec-2020 / 11:28 | Run Time:        | 43,00  |

| No.    | Time min | Peak Name | Peak Type | Area $\mu\text{S} \cdot \text{min}$ | Height $\mu\text{S}$ | Amount mg/L |
|--------|----------|-----------|-----------|-------------------------------------|----------------------|-------------|
| 2      | 27,52    | Fumarate  | BMB       | 30,875                              | 44,942               | n.a.        |
| TOTAL: |          |           |           | 30,88                               | 44,94                | 0,0         |

