This report has been prepared with the financial support of the Prevention of and Fight against Crime Programme of the European Union (grant agreement number JUST/2013/ISEC/DRUGS/AG/6413). The contents of this report are the sole responsibility of the National Forensic Laboratory and can in no way be taken to reflect the views of the European Commission.

Acknowledgement: Sample (not NMR confirmed) was kindly provided by the Institute of Forensic Medicine, University of Freiburg, Germany. Analytical data shown in this report were provided by NFL and FKKT, Slovenia.

Created by OPSIN free tool: http://opsin.ch.cam.ac.uk/ DOI: 10.1021/ci100384d
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 6.1 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 4 cm⁻¹

4. GC-(MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)
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>CH₂Cl₂</td>
<td>soluble</td>
</tr>
<tr>
<td>MeOH</td>
<td>partially</td>
</tr>
<tr>
<td>H₂O</td>
<td>partially</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): 21,95  
                       |         | BP(1): 334; BP(2): 409, BP(3): 127, |
| HPLC-TOF            | +       | Exact mass (theoretical): 409,1824; measured value Δppm: 0,01; formula: C₂₈H₂₄FNO₄ |
| FTIR-ATR            | +       | direct measurement (sample as received) |
| FTIR (condensed phase) always as base form | + | |
| IC (anions)         | +       | |
| NMR (in FKKT)       | +       | |
| validation          |         | MS spectrum consistent with the one published in ENFSI 2016 and Caymans for EG-2201 |
| other               |         |         |
ANALYTICAL RESULTS

MS (EI)

Abundance

Scan 4044 (21.947 min): EG-2201_1461-16.D

m/z: 77.0, 127.0, 173.1, 207.0, 250.0, 282.1, 372.1, 334.1, 409.2

m/z -->
FTIR-ATR - direct measurement (sample as received)

IR (condensed phase – after chromatographic separation)

NOTE: This is condensed phase IR (per base form of substance)
TOF REPORT

Data File: EG-2201_1461-16_TOF.d
Sample Name: ID_1461-16
Sample Type: Sample
Position: P2-C3
Instrument Name: 6230B TOF LC-MS
User Name: TG
Acq Method: general-1512015-XDB-C18-ESI-poz-pod.m
Acquired Time: 2/23/2016 1:41:38 PM
IRM Calibration Status: Success
DA Method: Drugs_NFL.m

Comment: extract in MeOH

Compound Table

<table>
<thead>
<tr>
<th>Cpd</th>
<th>Compound Name</th>
<th>MFG Formula</th>
<th>Obs. RT</th>
<th>Obs. Mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>EG-2201</td>
<td>C28 H24 F N O</td>
<td>10.838</td>
<td>409.1842</td>
</tr>
</tbody>
</table>

Name | Obs. m/z | Obs. RT | Obs. Mass | DB RT | DB Formula | DB Mass | DB Mass Error (ppm)
--- | -------- | ------- | --------- | ----- | ---------- | ------- | ---------------------
EG-2201 | 410.1914 | 10.838 | 409.1842 | 10.84 | C28 H24 F N O | 409.1842 | 0.01

Compound Chromatograms

MFE MS Zoomed Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

<table>
<thead>
<tr>
<th>Obs. m/z</th>
<th>Charge</th>
<th>Abund</th>
<th>Formula</th>
<th>Ion/Isotope</th>
</tr>
</thead>
<tbody>
<tr>
<td>410.1914</td>
<td>1</td>
<td>5205565</td>
<td>C28 H24 F N O</td>
<td>(M+H)+</td>
</tr>
<tr>
<td>411.1949</td>
<td>1</td>
<td>1615425.24</td>
<td>C28 H24 F N O</td>
<td>(M+H)+</td>
</tr>
<tr>
<td>412.1992</td>
<td>1</td>
<td>237267.33</td>
<td>C28 H24 F N O</td>
<td>(M+H)+</td>
</tr>
<tr>
<td>432.1732</td>
<td>1</td>
<td>110992.23</td>
<td>C28 H24 F N O</td>
<td>(M+H)+</td>
</tr>
<tr>
<td>433.1764</td>
<td>1</td>
<td>32620.03</td>
<td>C28 H24 F N O</td>
<td>(M+Na)+</td>
</tr>
<tr>
<td>819.3746</td>
<td>1</td>
<td>80481.77</td>
<td>C28 H24 F N O</td>
<td>(2M+H)+</td>
</tr>
<tr>
<td>820.3778</td>
<td>1</td>
<td>47275.66</td>
<td>C28 H24 F N O</td>
<td>(2M+H)+</td>
</tr>
<tr>
<td>841.3574</td>
<td>1</td>
<td>228306.3</td>
<td>C28 H24 F N O</td>
<td>(2M+Na)+</td>
</tr>
<tr>
<td>842.3602</td>
<td>1</td>
<td>133928.09</td>
<td>C28 H24 F N O</td>
<td>(2M+Na)+</td>
</tr>
<tr>
<td>843.3635</td>
<td>1</td>
<td>37572.13</td>
<td>C28 H24 F N O</td>
<td>(2M+Na)+</td>
</tr>
</tbody>
</table>

--- End Of Report ---
## Peak Integration Report

<table>
<thead>
<tr>
<th>No.</th>
<th>Time (min)</th>
<th>Peak Name</th>
<th>Peak Type</th>
<th>Area (µS·min)</th>
<th>Height (µS)</th>
<th>Amount (n.a.)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TOTAL:</td>
<td></td>
<td></td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

### Graph

![Graph showing peak integration](attachment:image.png)

**Sample Name:** EG-2201_1461-16_IC  
**Injection Vol.:** 25.00  
**Injection Type:** Unknown  
**Dilution Factor:** 1.0000  
**Program:** ANIONI  
**Operator:** kemija  
**Inj. Date / Time:** 24-Jun-2016 / 21:48  
**Run Time:** 42.00
REPORT

Sample ID: 1461-16

Our notebook code: P-1461-16

NMR sample preparation: 15 mg dissolved in 0.7 mL CDCl₃

NMR experiments: ¹H, ¹³C, ¹H⁻¹H gs-COSY, ¹H⁻¹³C gs-HSQC, ¹H⁻¹³C gs-HMBC, ¹H⁻¹⁵N gs-HMBC.

Proposed structure:

Chemical name: (9-(5-fluoropentyl)-9H-carbazol-3-yl)(naphthalen-1-yl)methanone

Comments: - Structure elucidation based on 1D and 2D NMR spectra
- Sample contains some minor impurities, as evident from NMR.

Supporting information: Copies of ¹H and ¹³C NMR spectra

Author: Prof. Dr. Janez Košmrlj, Doc. Dr. Krištof Kranjc

Date of report: October 19, 2016

This report has been produced with the financial support of the Prevention of and Fight against Crime Programme of the European Union (grant agreement number JUST/2013/ISEC/DRUGS/AG/6413). The contents of this publication are the sole responsibility of the Author and can in no way be taken to reflect the views of the European Commission.
Current Data Parameters
NAME          P-1461-16
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20160817
Time               0.50
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 5120
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            0.454131 Hz
RG                 2050
DW               16.800 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

-------- CHANNEL f1 --------
SFO1        125.7703637 MHz
NUC1                13C
P1                 9.00 usec
PLW1       122.00000000 W
PLW12        0.32179001 W
PLW13        0.16186000 W

F2 - Processing parameters
SI                32768
SF          125.7577907 MHz
WDW                  EM
SSB      0
LB                 1.00 Hz
GB                 0
PC                 1.00