

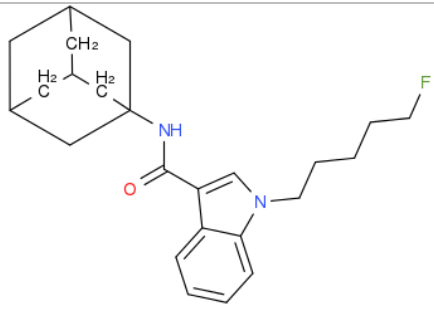
## ANALYTICAL REPORT

### STS-135 (C<sub>24</sub>H<sub>31</sub>FN<sub>2</sub>O)

#### N-(Adamantan-1-yl)-1-(5-fluoropentyl)-1H-indole-3-carboxamide

Remark – other NPS detected: **none**

|                     |                      |
|---------------------|----------------------|
| Sample ID:          | 1200-15              |
| Sample description: | powder - white       |
| Sample type:        | test purchase        |
| Comments:           | RESPONSE -purchasing |
| Date of entry:      | 7/29/2015            |

|   |   |
|---|---|
| Substance identified-structure <sup>i</sup> (base form) |  |
| Systematic name   | N-(Adamantan-1-yl)-1-(5-fluoropentyl)-1H-indole-3-carboxamide                       |
| Other names   | STS-135   |
| Formula (per base form)                                 | C <sub>24</sub> H <sub>31</sub> FN <sub>2</sub> O                                   |
| M <sub>w</sub> (g/mol)                                  | 382,5   |
| Salt form   | base  |
| Smiles  | C12(CC3CC(CC(C1)C3)C2)NC(=O)C2=CN(C3=CC=CC=C3)CCCCCF                                |
| Compound Class  | Cannabinoids  |
| Other NPS detected                                      | none  |
| Add.info (purity..)                                     | pure  |

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## Supporting information

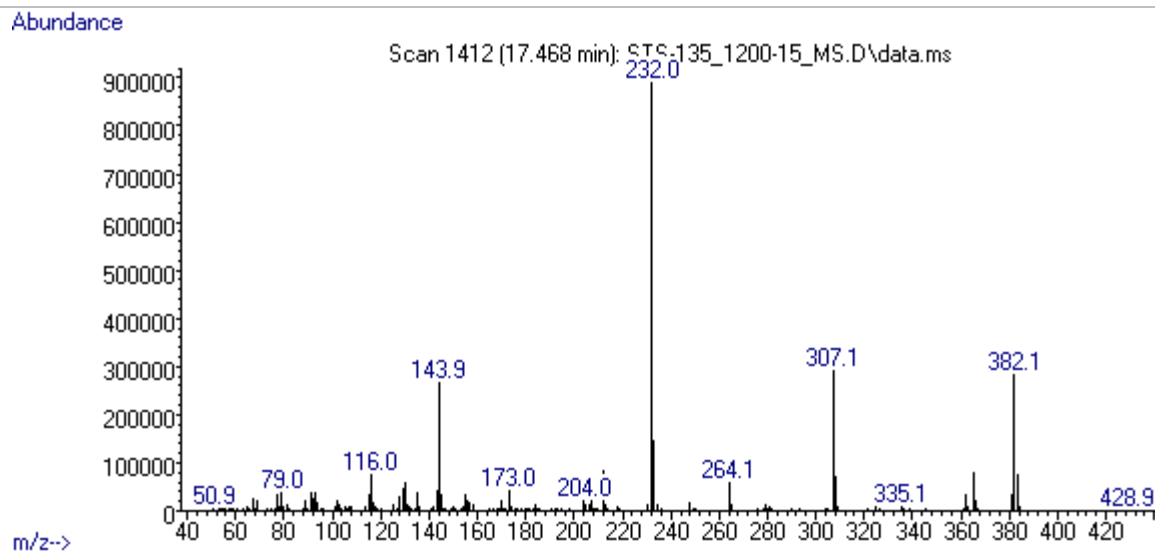
| Analytical technique:                         | applied | remarks  |
|---|---------|--|
| GC-MS (EI ionization)                         | +       | NFL GC-RT (min): 17,47<br>BP(1): 232; BP(2): 382,BP(3) :144,   |
| FTIR-ATR                                      | +       | direct measurement   |
| FTIR (condensed phase)<br>always as base form | -       |  |
| HPLC-TOF                                      | +       | Exact mass (theoretical): 382,242;<br>measured value $\Delta$ ppm:0,03;<br>formula:C <sub>24</sub> H <sub>31</sub> FN <sub>2</sub> O |
| NMR-confirmed                                 | -       |  |
| validation                                    |         | FTIR ATR spectrum consistent by SWGDRUG spectrum of STS-135(Lot#0436854-17); corelation 0,99   |
| other   |         | sample completely soluble in CH <sub>2</sub> CL <sub>2</sub> and in MeOH   |

GC-MS (Agilent): GC-method is RT locked to tetracosane (RT=9.53 min). Injection volume 1 ml and split mode (1:50)for GC-MS instruments and 1:5 for GC-MS-FTIR(condensed phase). Injector temperature: 280 °C. Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 mm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, than heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadropole temperatures 280°C and 180°C. m/z scan range: from 50 (40) to 550 amu.

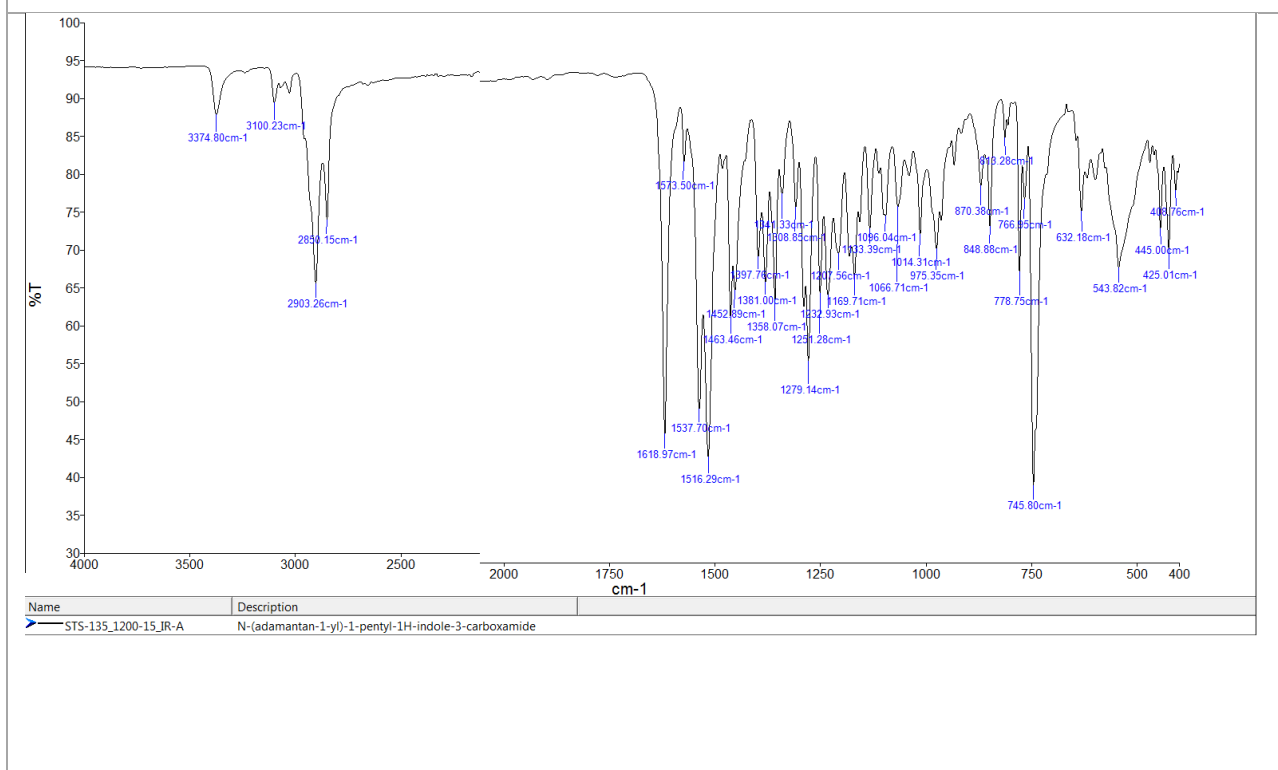
FTIR-ATR (Perkin Elmer): scan range 4000-400 cm<sup>-1</sup>; resolution 4cm<sup>-1</sup>

FTIR (Spectra analyses-Danny): scan range 4000 to 700, resolution 4cm<sup>-1</sup>

## MS spectrum (EI)



## FTIR - ATR



<sup>i</sup> Created by OPSIN free tool: <http://opsin.ch.cam.ac.uk/> DOI: 10.1021/ci100384d

# Target Compound Screening Report

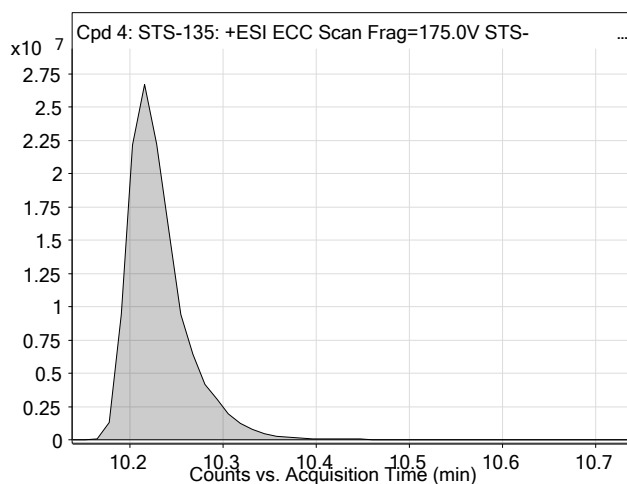
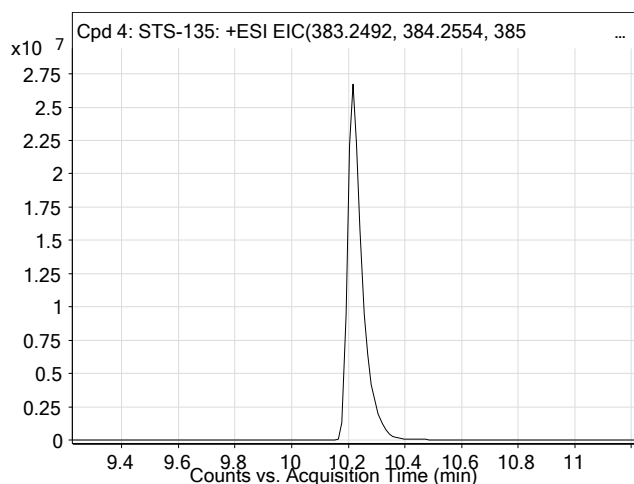
|                               |   |                      |                       |
|-------------------------------|---|----------------------|-----------------------|
| <b>Data File</b>              | STS-135_1200-15_TOF.d                     | <b>Sample Name</b>   | STS-135               |
| <b>Sample Type</b>            | Sample                                    | <b>Position</b>      | P1-D9                 |
| <b>Instrument Name</b>        | 6230B TOF LC-MS                           | <b>User Name</b>     | TG                    |
| <b>Acq Method</b>             | droge general-13-5-2015-XDB-C18-ESI-poz.m | <b>Acquired Time</b> | 7/27/2015 12:22:01 PM |
| <b>IRM Calibration Status</b> | Success                                   | <b>DA Method</b>     | Droge_Default.m       |
| <b>Comment</b>                | extract in MeOH                           |                      |                       |

## Compound Table

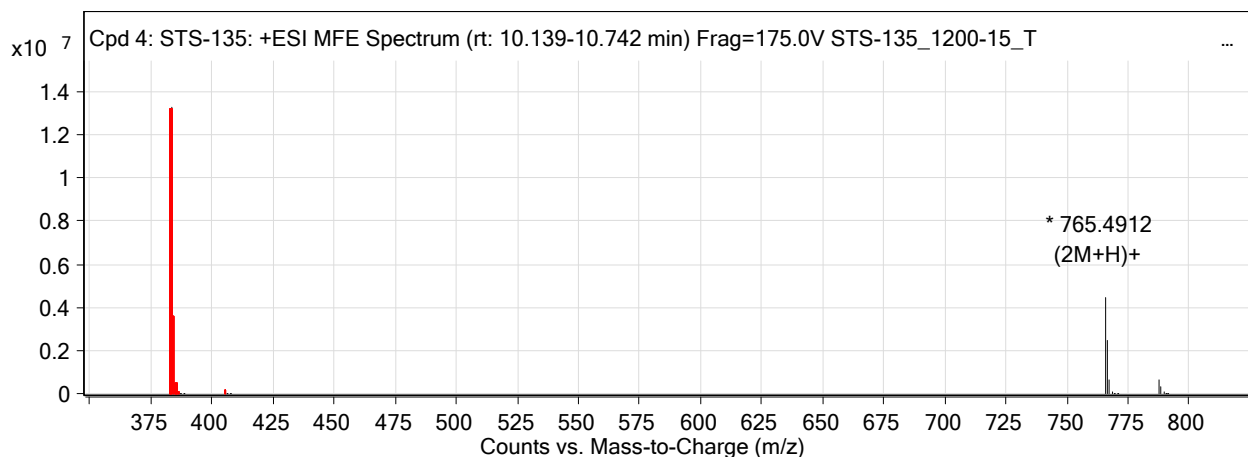
| Label          | Tgt Name | MFG Formula    | Obs. RT | Obs. Mass |
|----------------|----------|----------------|---------|-----------|
| Cpd 4: STS-135 | STS-135  | C24 H31 F N2 O | 10.22   | 382.242   |

| Name    | Obs. m/z | Obs. RT | Obs. Mass | DB RT  | DB Formula     | DB Mass | DB Mass Error (ppm) | Find Cpd Algorithm        |
|---------|----------|---------|-----------|--------|----------------|---------|---------------------|---------------------------|
| STS-135 | 383.2493 | 10.22   | 382.242   | 10.222 | C24 H31 F N2 O | 382.242 | 0.03                | Find by Molecular Feature |

## Compound Chromatograms



## MFE MS Zoomed Spectrum



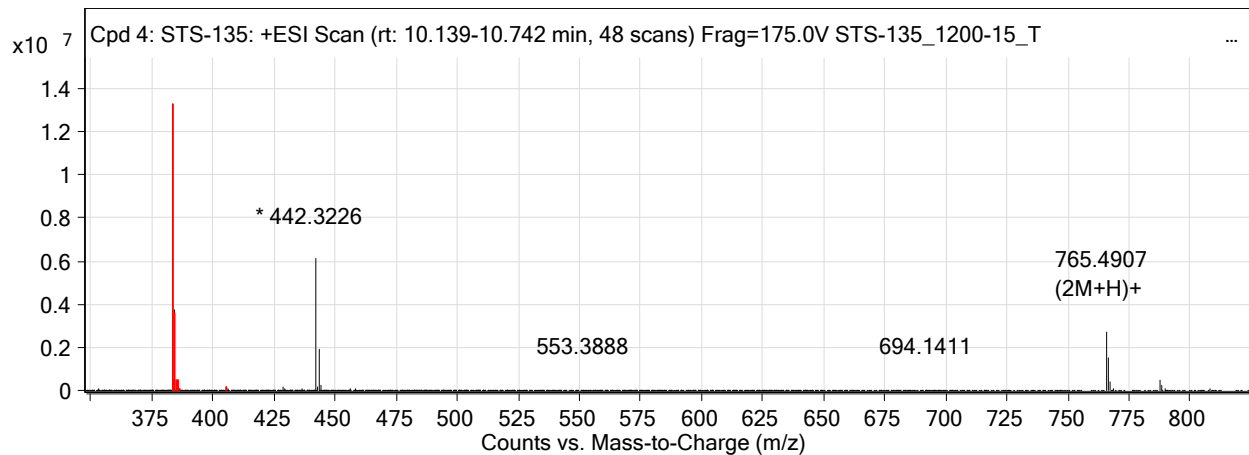
## MS Spectrum Peak List

| Obs. m/z | Charge | Abund      | Formula        | Ion/Isotope |
|----------|--------|------------|----------------|-------------|
| 383.2493 | 1      | 13291451   | C24 H31 F N2 O | (M+H)+      |
| 384.2526 | 1      | 3511238.26 | C24 H31 F N2 O | (M+H)+      |
| 385.2563 | 1      | 439861.82  | C24 H31 F N2 O | (M+H)+      |
| 405.2314 | 1      | 145958.19  | C24 H31 F N2 O | (M+Na)+     |
| 765.4912 | 1      | 4481838.5  |                | (2M+H)+     |
| 766.4946 | 1      | 2458185.89 |                | (2M+H)+     |
| 767.4982 | 1      | 650400.99  |                | (2M+H)+     |

# Target Compound Screening Report

|          |   |           |          |
|----------|---|-----------|----------|
| 768.5009 | 1 | 109537.66 | (2M+H)+  |
| 787.4736 | 1 | 644138.38 | (2M+Na)+ |
| 788.4767 | 1 | 338019.23 | (2M+Na)+ |

MS Zoomed Spectrum



--- End Of Report ---