GCMS Analytical Information

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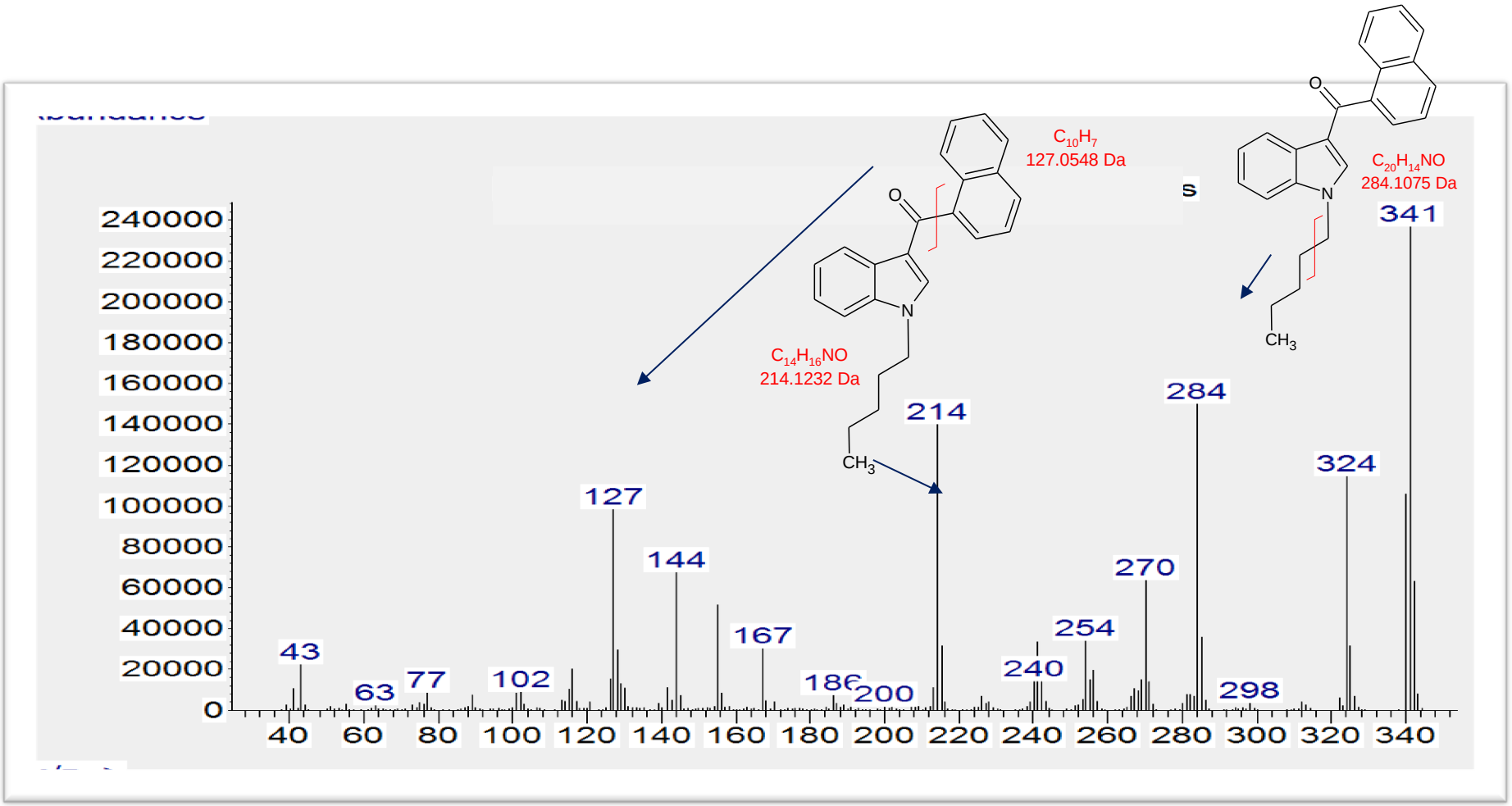
Goals

- GCMS Fragmentation
  - Nitrogen Rule
  - Isotope ratios
  - Synthetic cannabinoid fragmentation patterns
- Cyclopropyls
  - Ring-opened products
- URB597
- Isomers
  - JWH Methoxy isomers
  - AM2201 isomers
  - Azepene/Azepane
- Derivitization
  - Fluoromethamphetamine isomers
  - UR144 – ring opened – alcohol
- PB-22

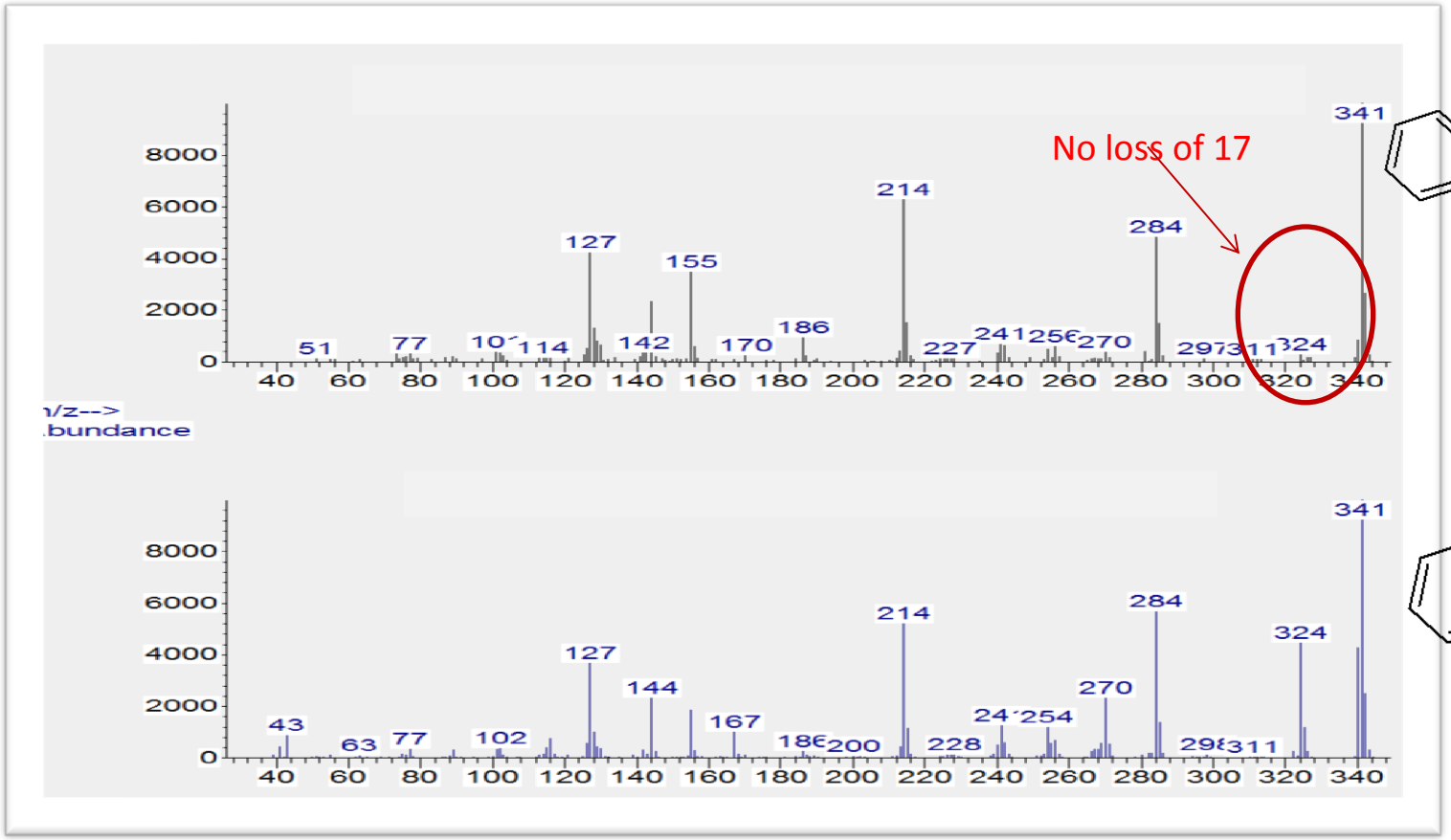
GCMS Fragmentation

- Fragmentation can be predicted to occur at the site with the lowest ionization energy
- Nitrogen Rule
  - A compound with an even molecular weight will have zero or an even number of nitrogens
  - A compound with an odd molecular weight will have an odd number of nitrogens
- Isotope ratios (M:M+2)
  - Chlorine – 3:1
  - Bromine – 1:1

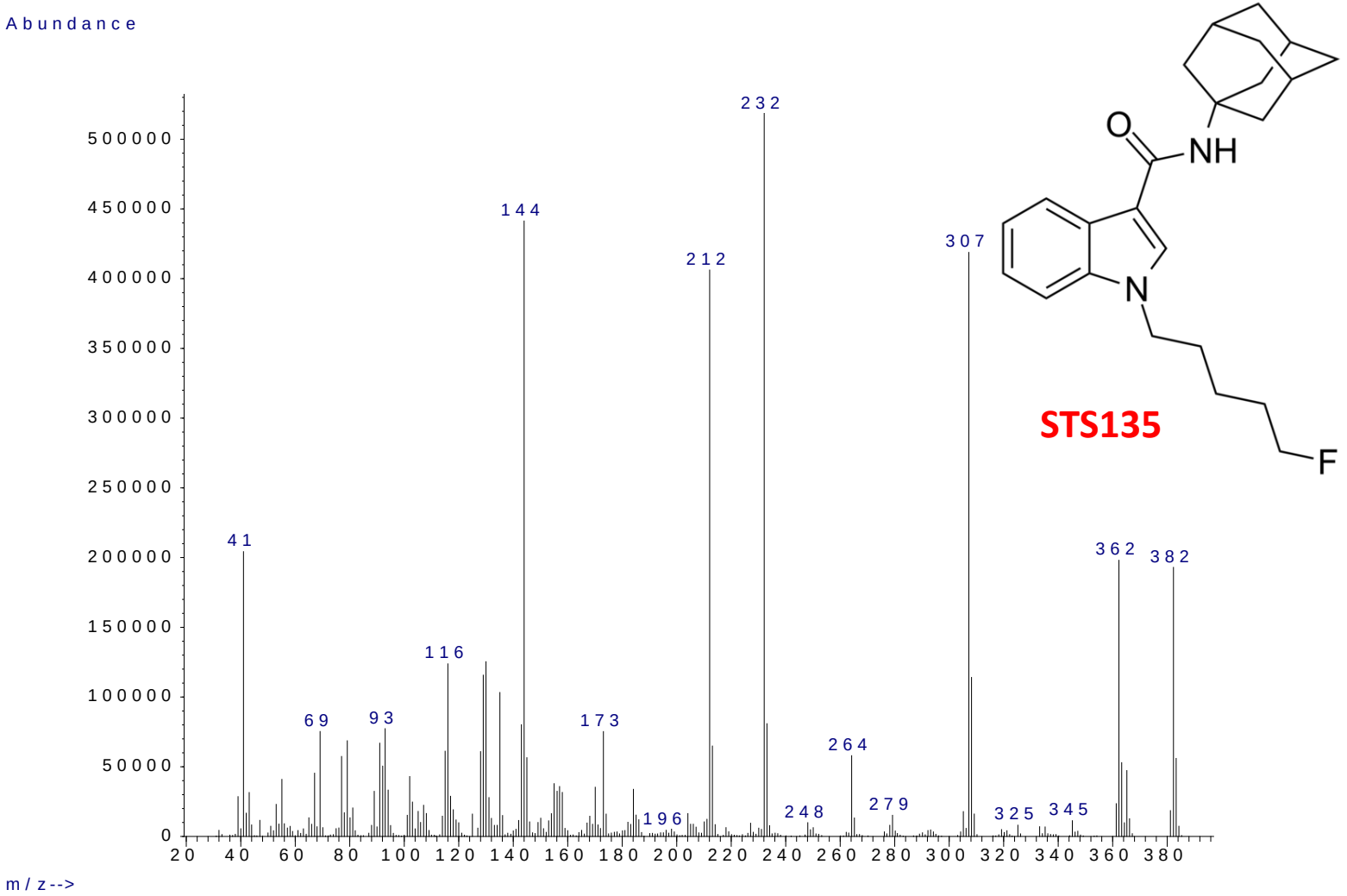
JWH-018 Fragmentation



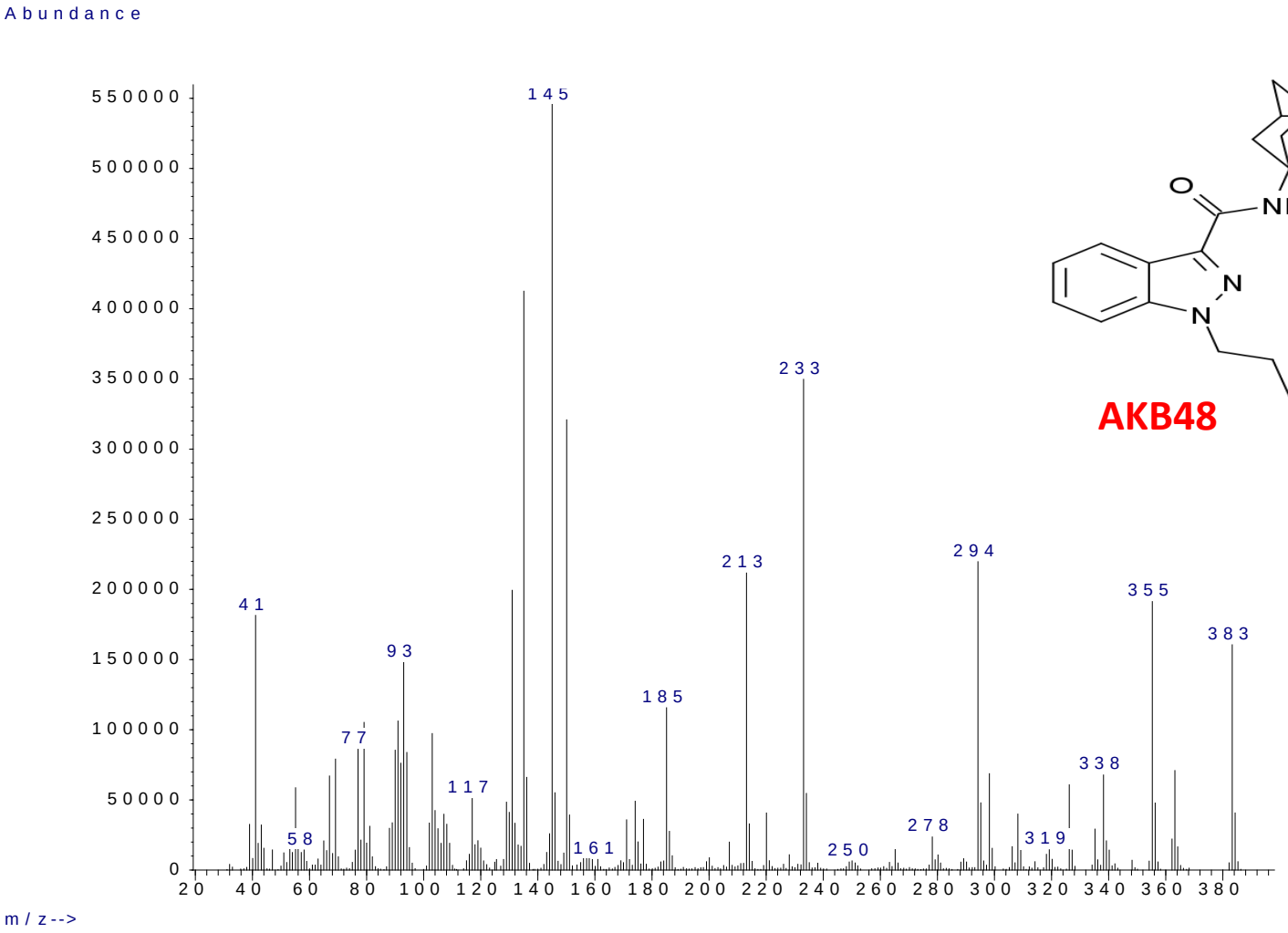
2 vs. 1-Naphthyl Isomer of JWH-018



Indole vs. Indazole

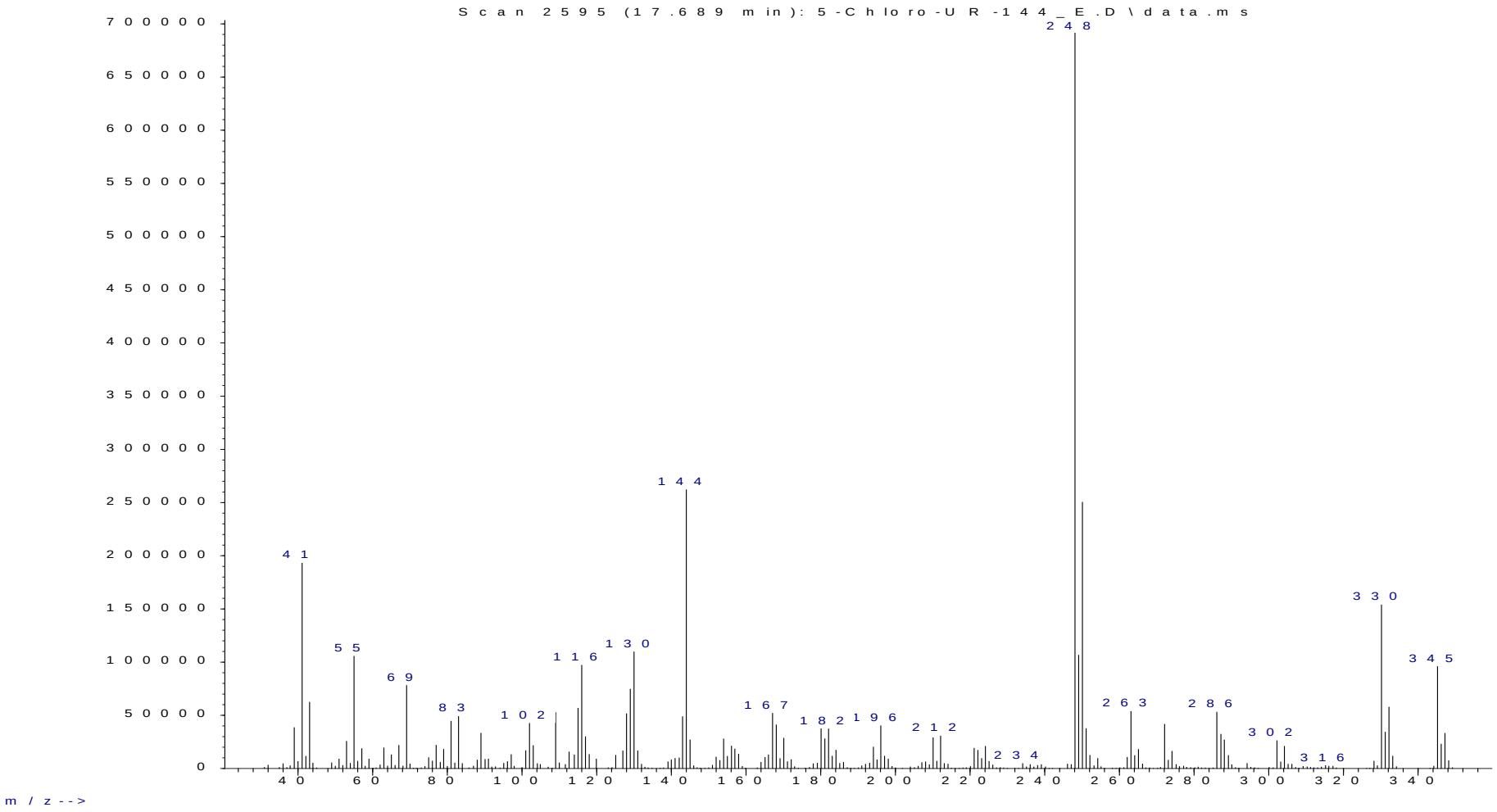


Indole vs. Indazole

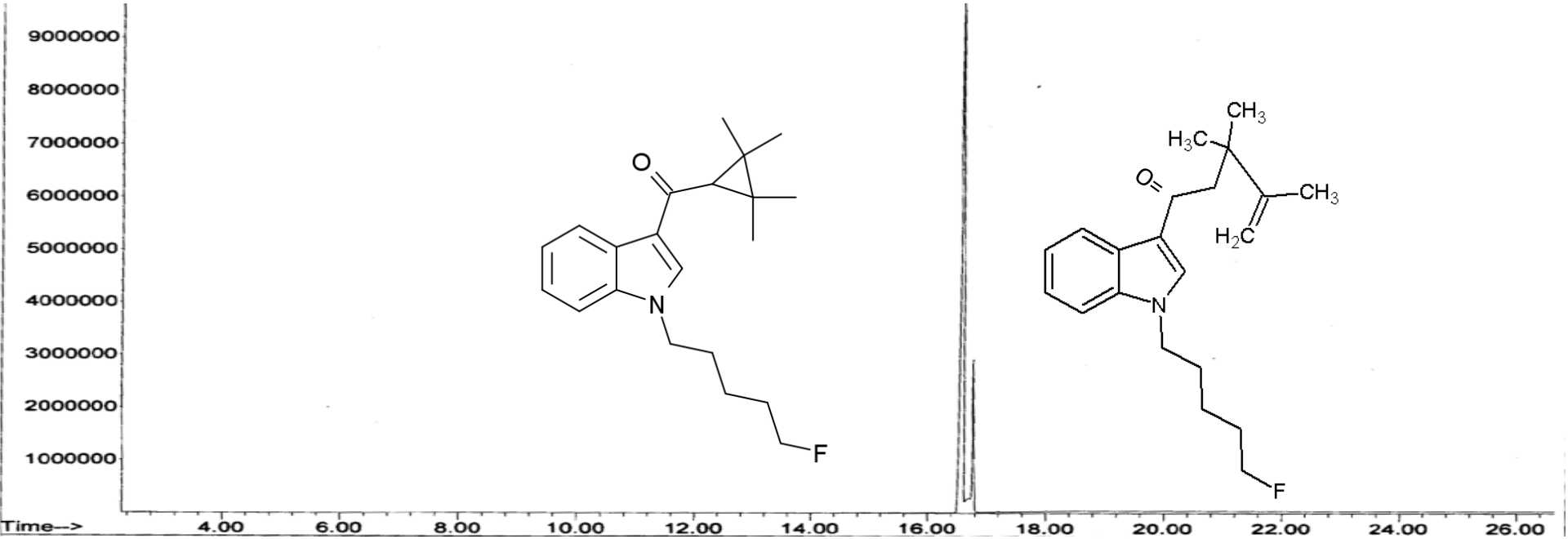


AKB48

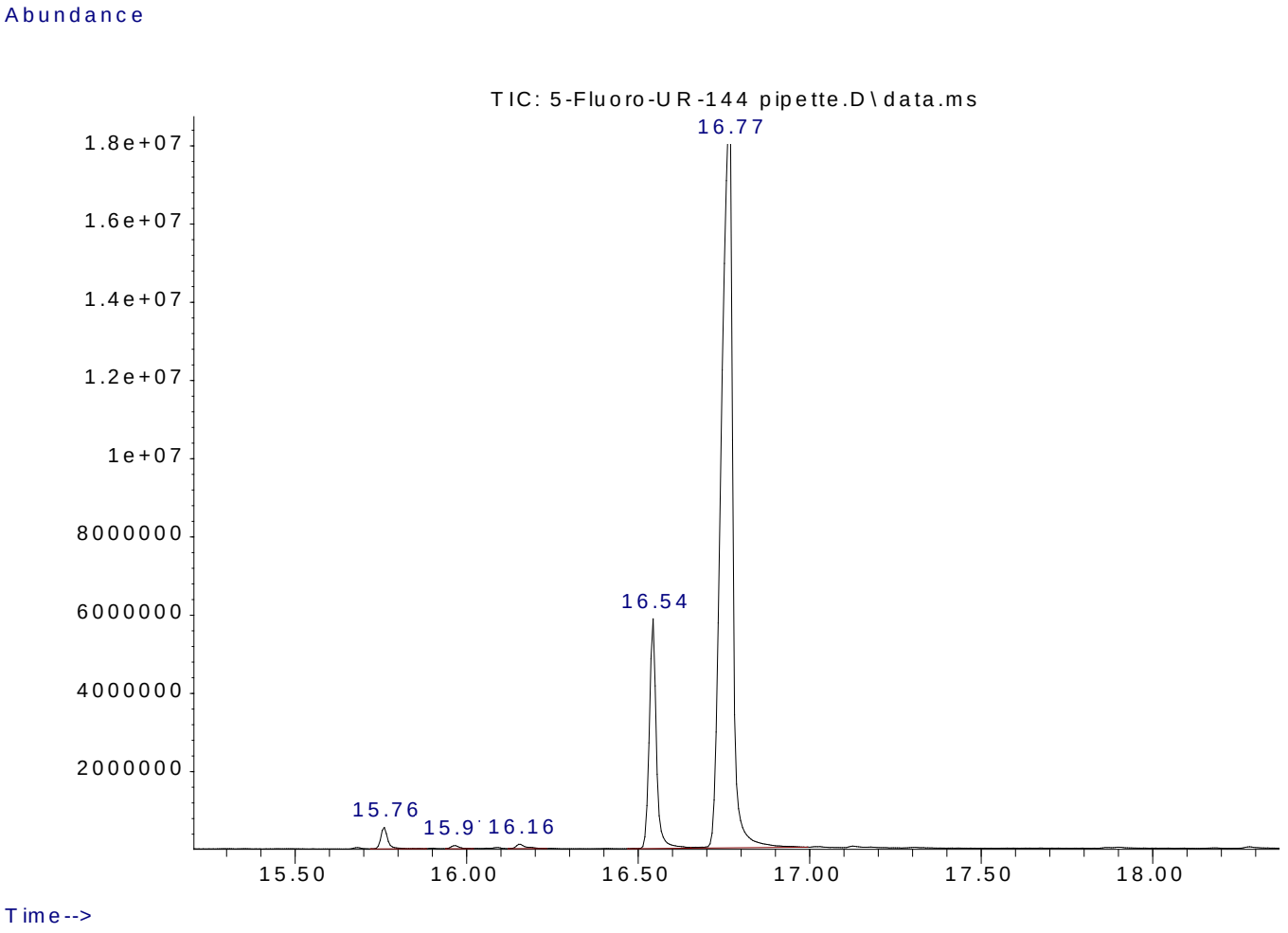
Chloro-UR144



Cyclopropyl Rearrangement



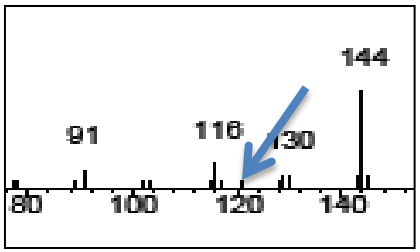
Smoking Experiment



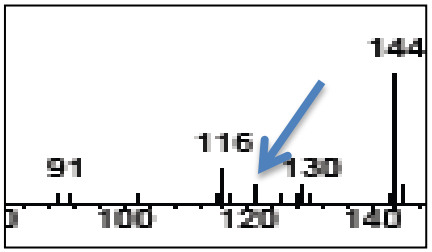
JWH-250, -302, -201

Focus on the 121:91 ion ratio (use tabulate in Chemstation).

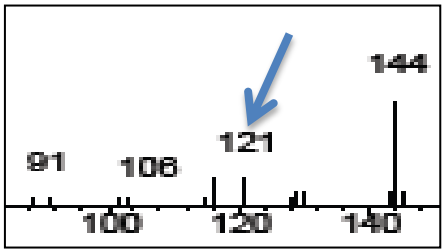
JWH-250



JWH-302



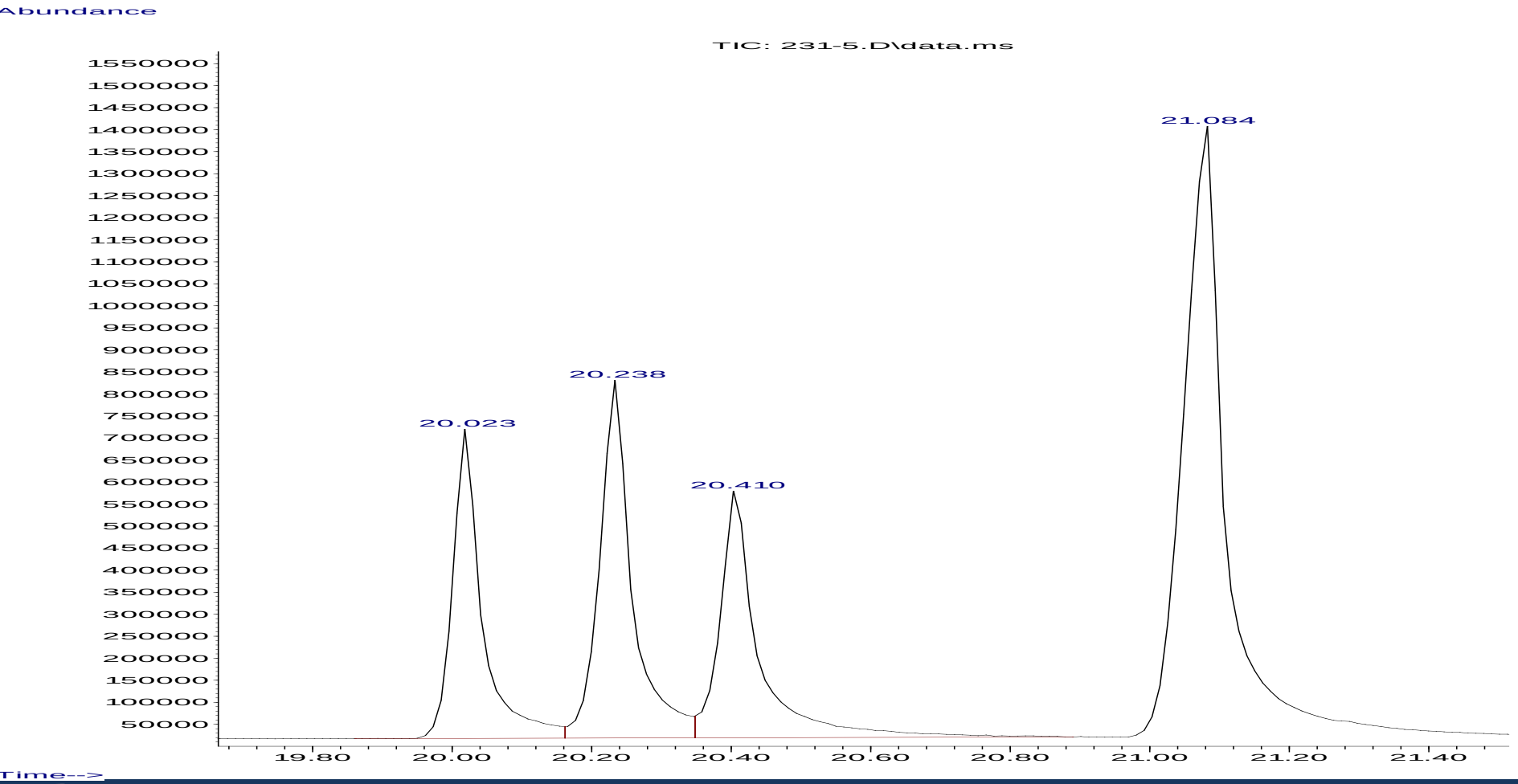
JWH-201



Compound	Ratio
JWH-250	0.4
JWH-302	1.3
JWH-201	7.2

Harris, D.; Hokanson, S.; Miller, V. "*GC–MS Differentiation of Three Synthetic Cannabinoid Positional Isomers: JWH–250, JWH–302, and JWH–201*." CLIC Journal, October 2011, 21(4), 23-32.

AM2201 Isomers

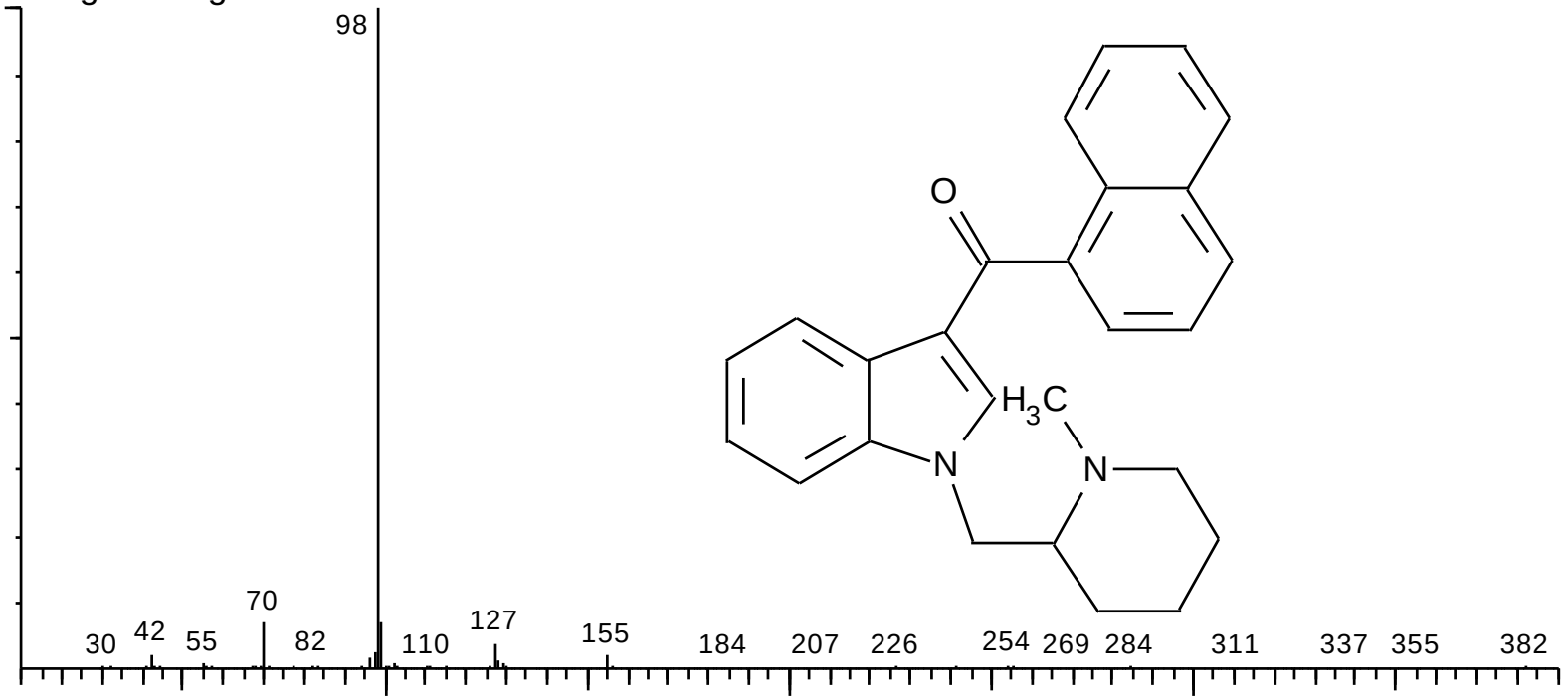


AM1220

AM-1220

1-((N-Methylpiperidin-2-yl)methyl)-3-(1-naphthoyl)indole

Designer drug



MW:382.50532

MM:382.20451

$C_{26}H_{26}N_2O$

RI:3482 (SE-30)

GC/MS

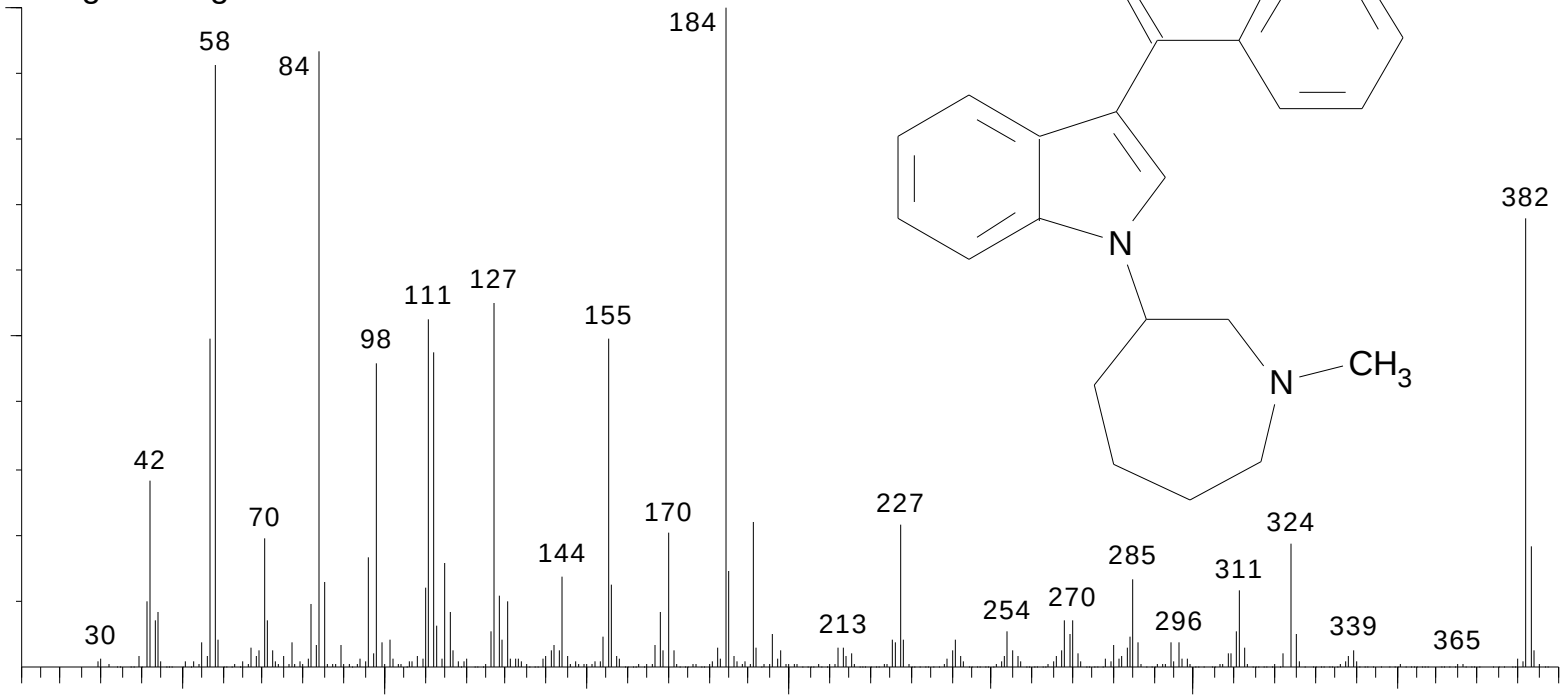
EI 70 eV

TSQ 7000

QI:996, IMM

AM1220 Azepane Isomer

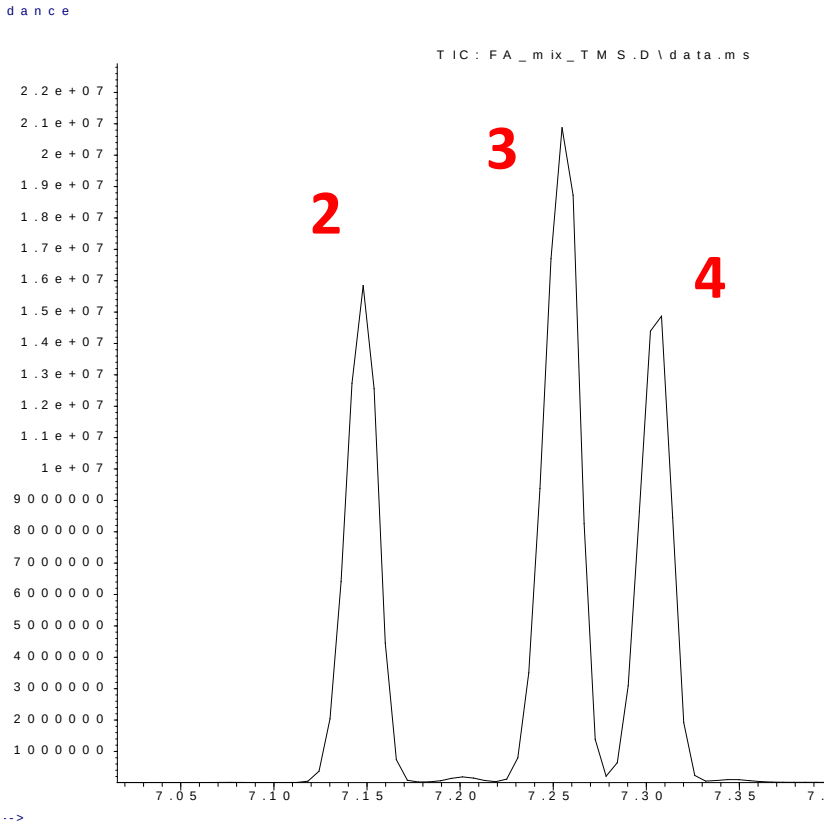
AM-1220 (azapane isomer)
1-(N-Methylazepan-3-yl)-3-(1-naphthoyl)indole
Designer drug

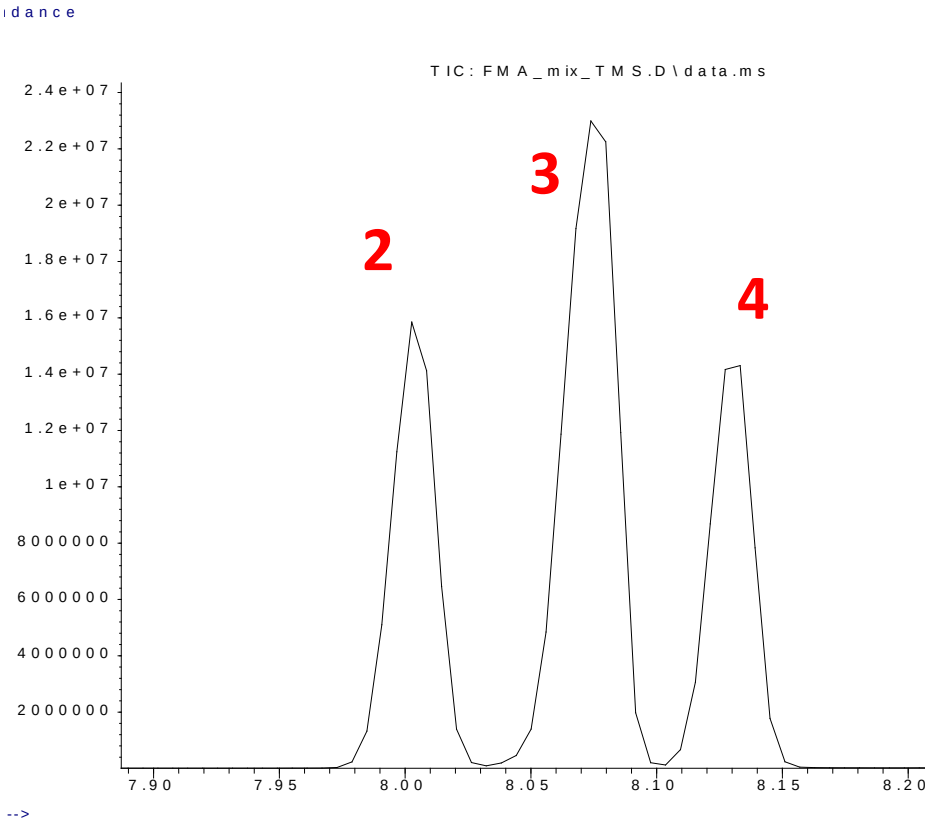


MW:382.50532
MM:382.20451
$C_{26}H_{26}N_2O$
RI:3481 (SE-30)

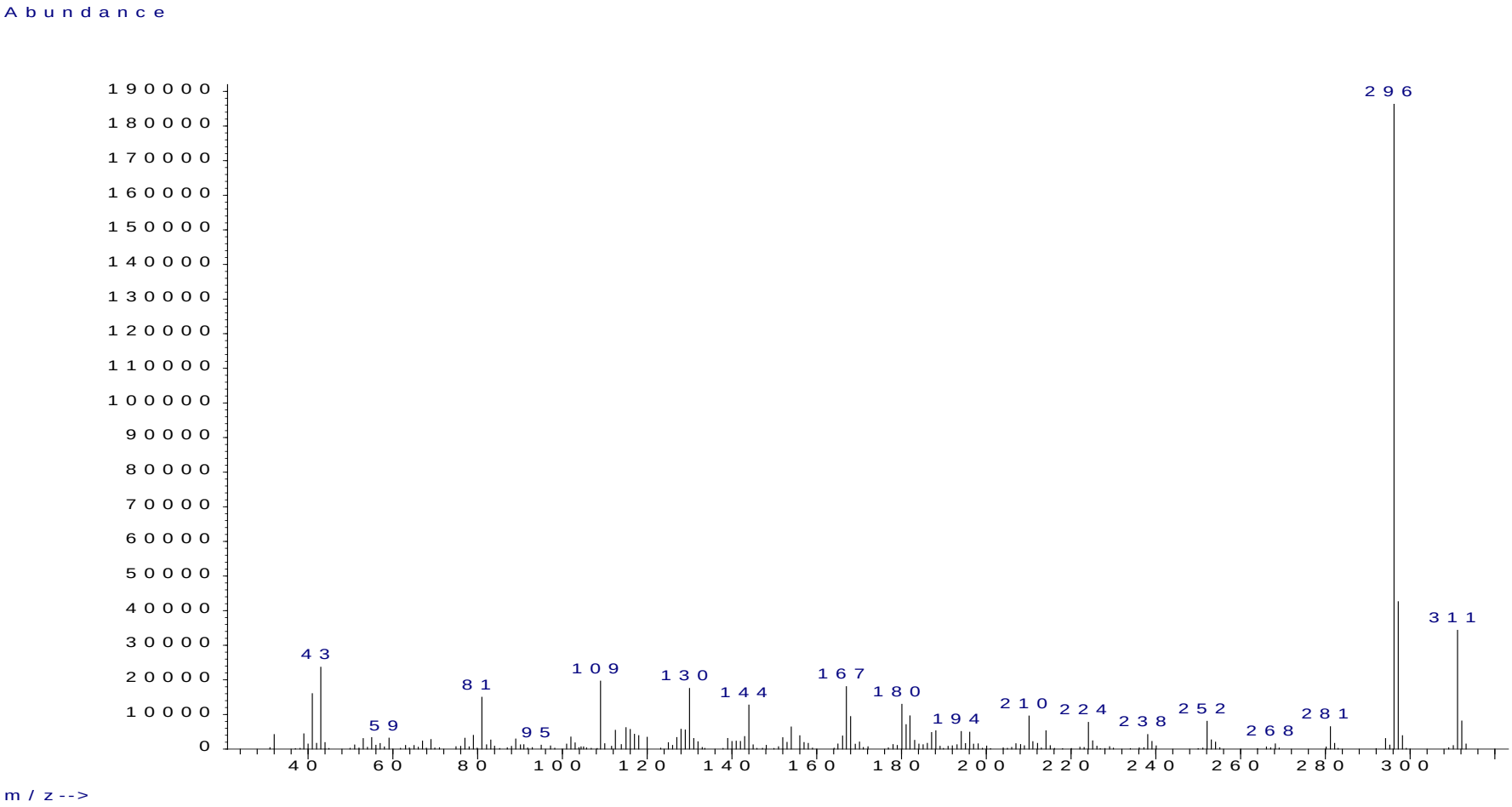
GC/MS
EI 70 eV
TSQ 7000
QI:996

Fluoro Isomers

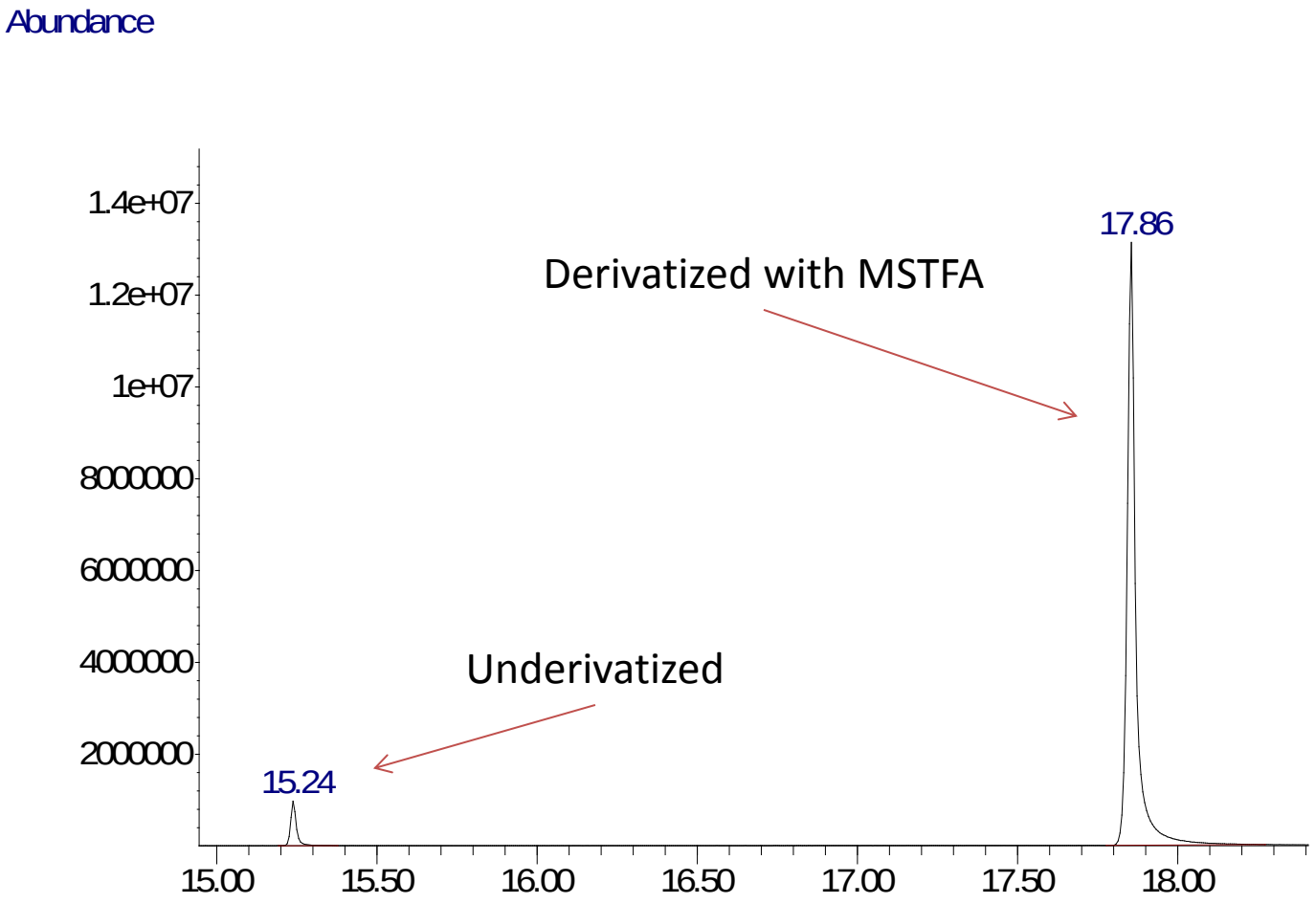




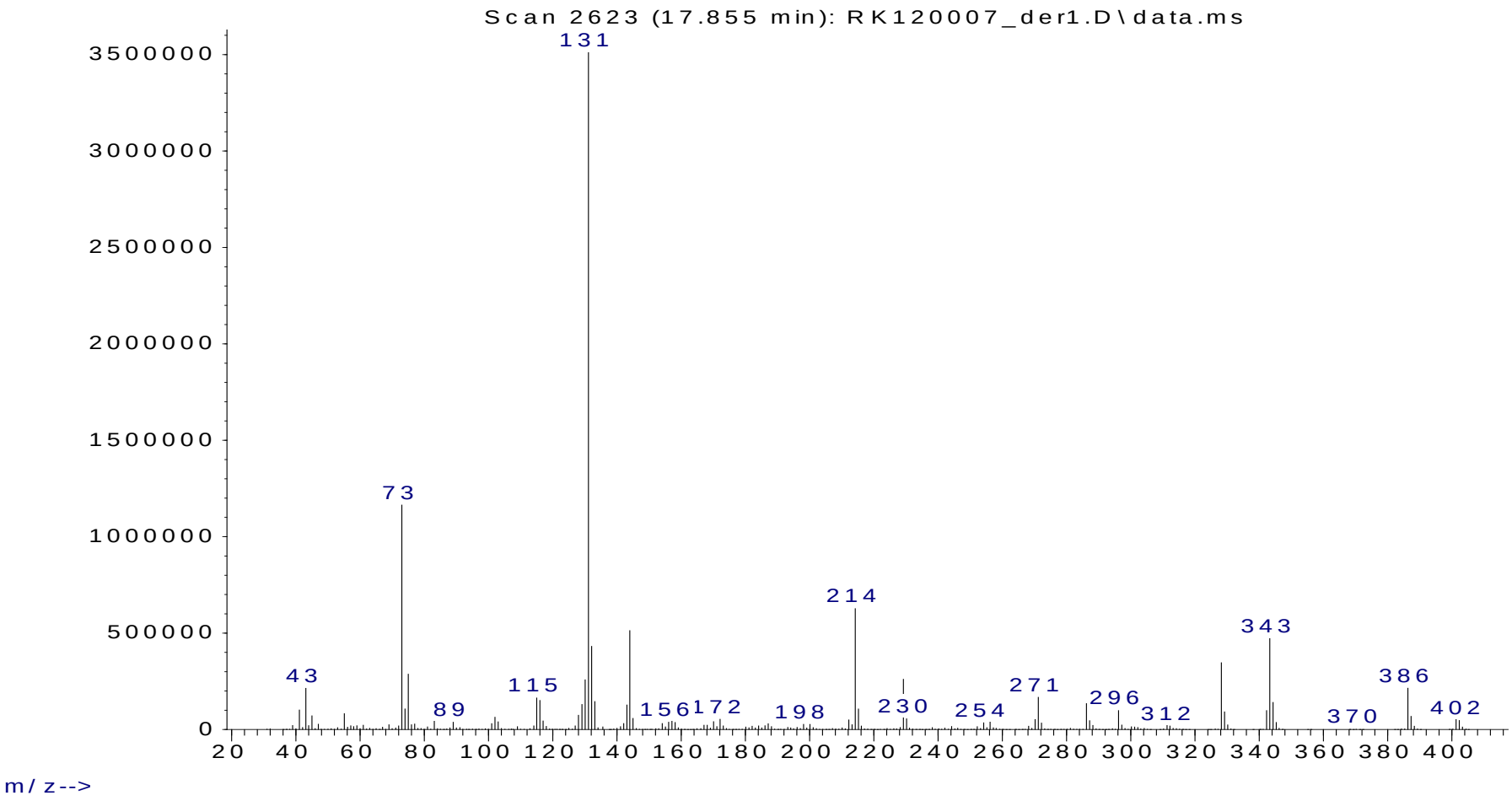
Unknown UR144 Related Compound



Unknown UR144 Related Compound

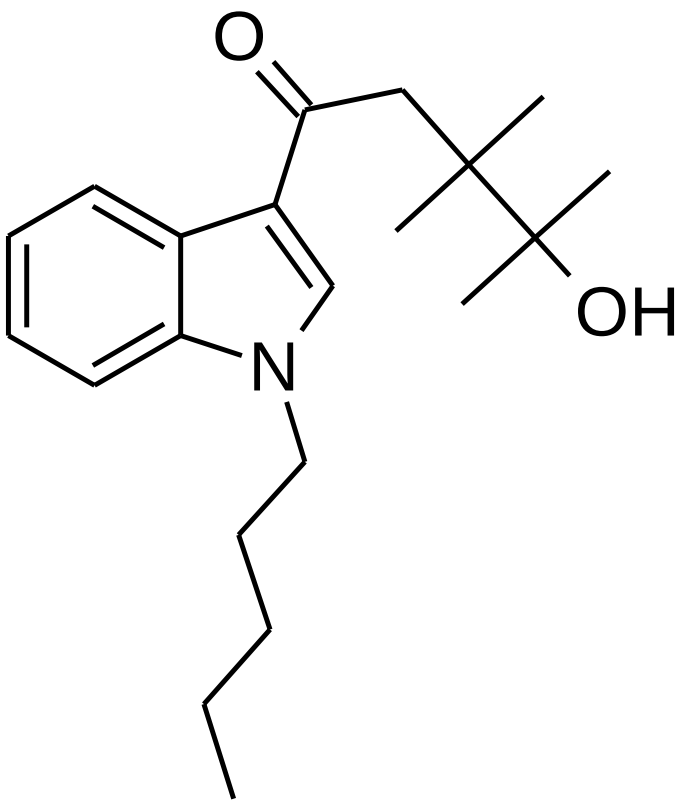


Unknown UR144 Related Compound

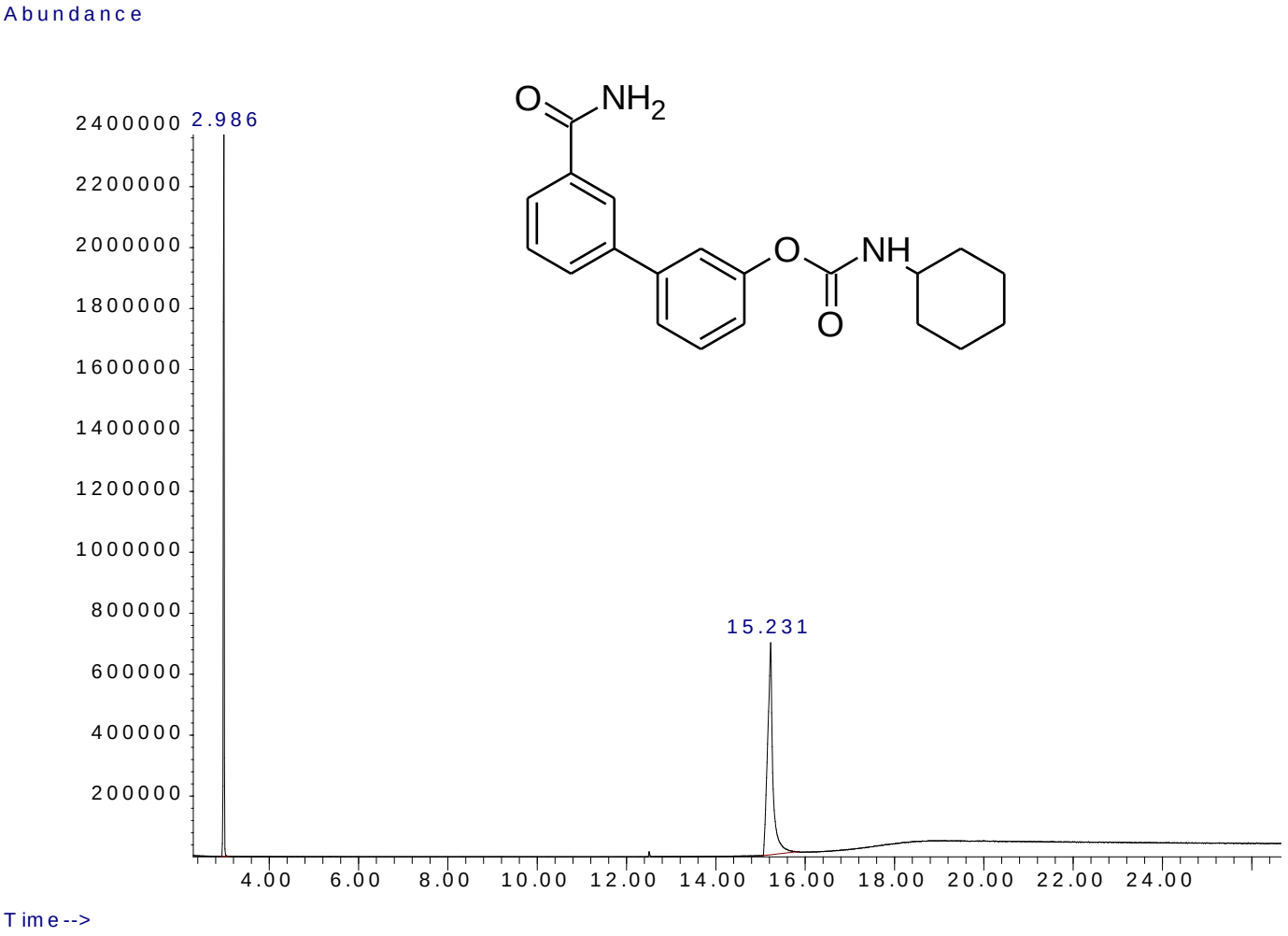


Unknown UR144 Related Compound

- "UR-144 in products sold via the Internet: Identification of related compounds and characterization of pyrolysis products", Andrej Grigoryev, Et al. **Drug Testing and Analysis**, January 2013
- "Identification and analytical properties of new synthetic cannabimimetics bearing 2,2,3,3-tetramethylcyclopropanecarbonyl moiety", Yuri Shafran, Et al. **Forensic Science International**, 2012

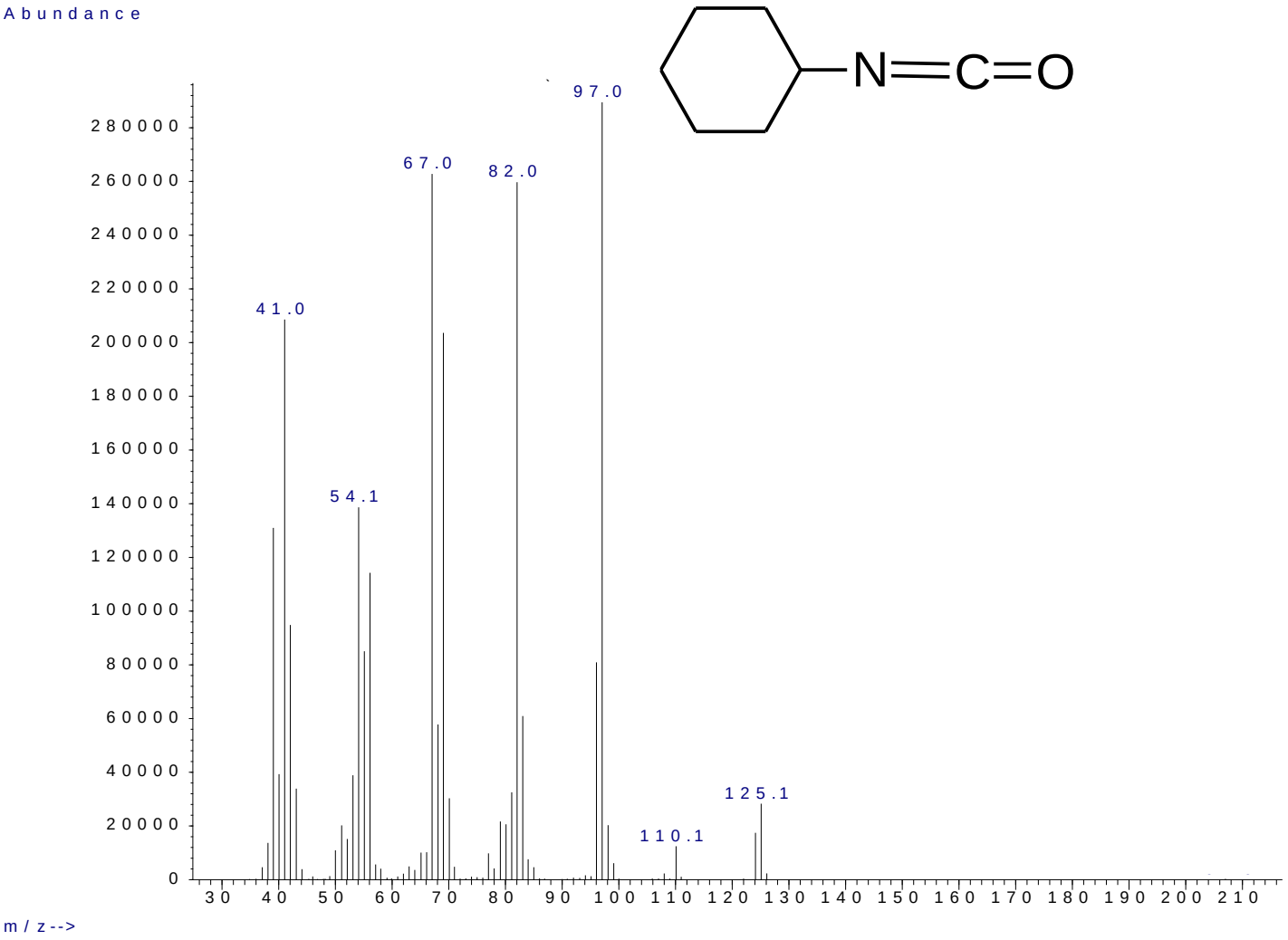


URB597


Abundance
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
2.986
15.231
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00
Time-->

O
NH2
O
NH
O

URB597


Abundance
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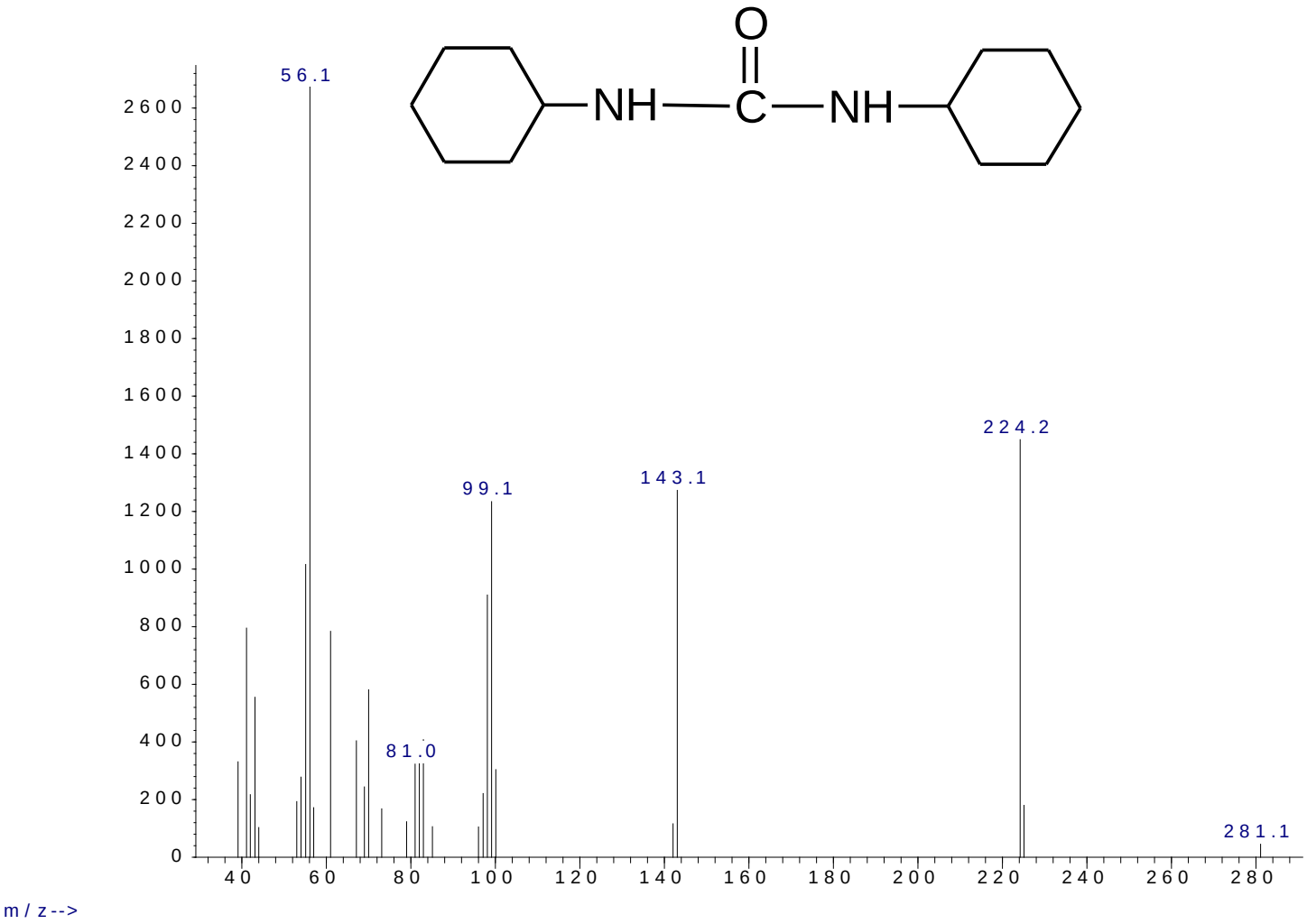
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
97.0
67.0
82.0
41.0
54.1
125.1
110.1
30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210
m/z-->

N=C=O

URB597


Abundance
O
NH
C
NH
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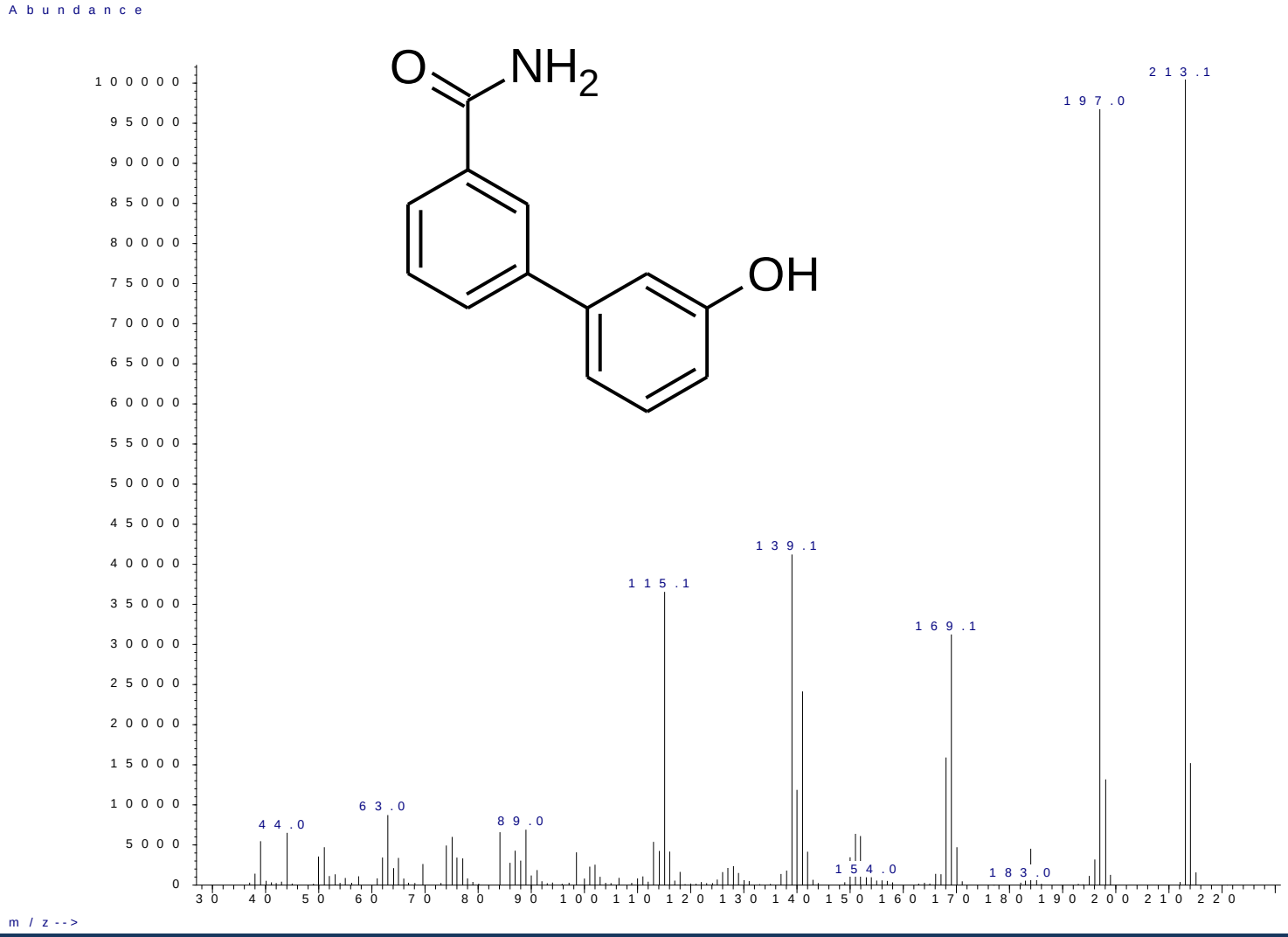
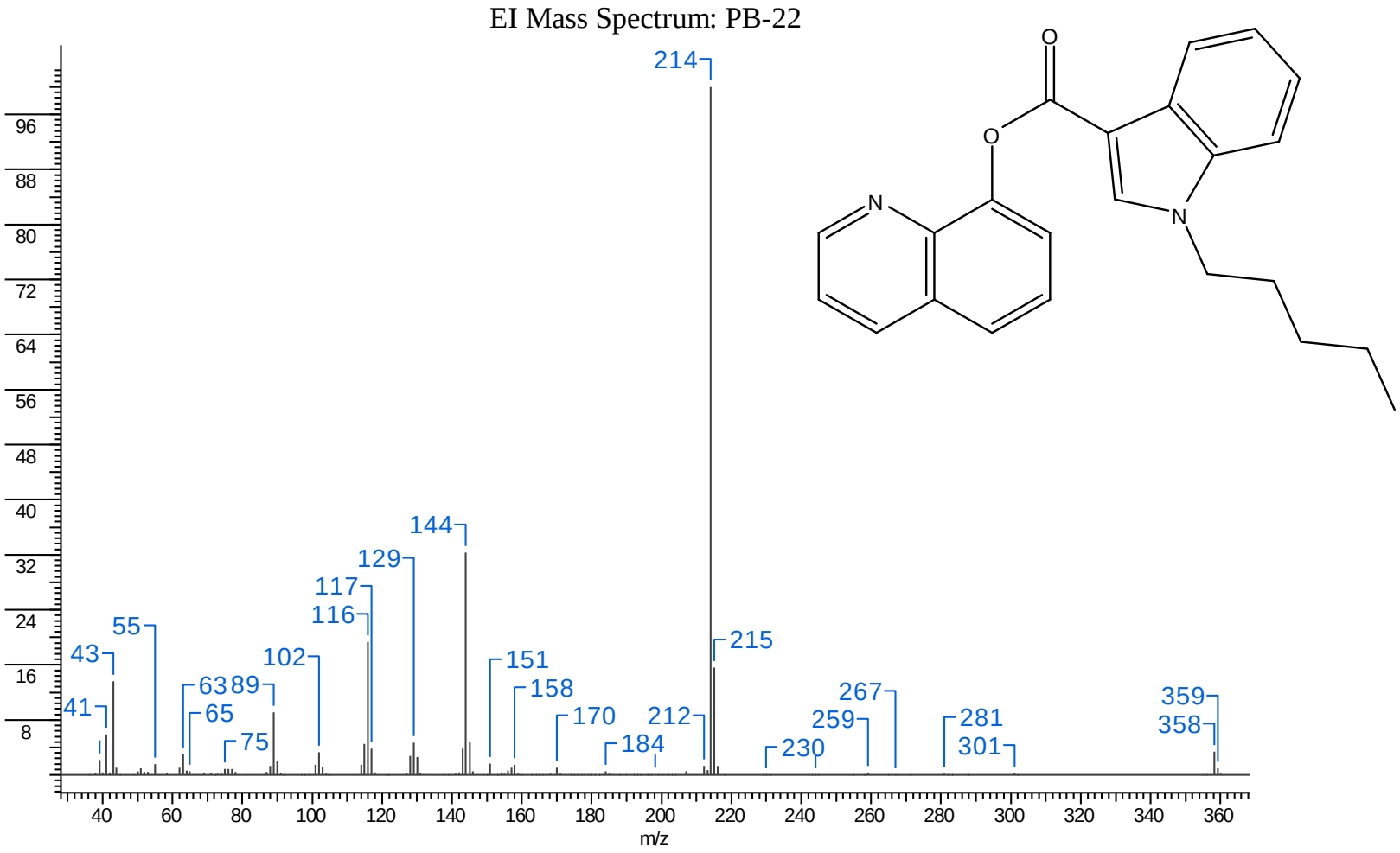
99.1
81.0
143.1
224.2
281.1
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
40
60
80
100
120
140
160
180
200
220
240
260
280
m/z-->

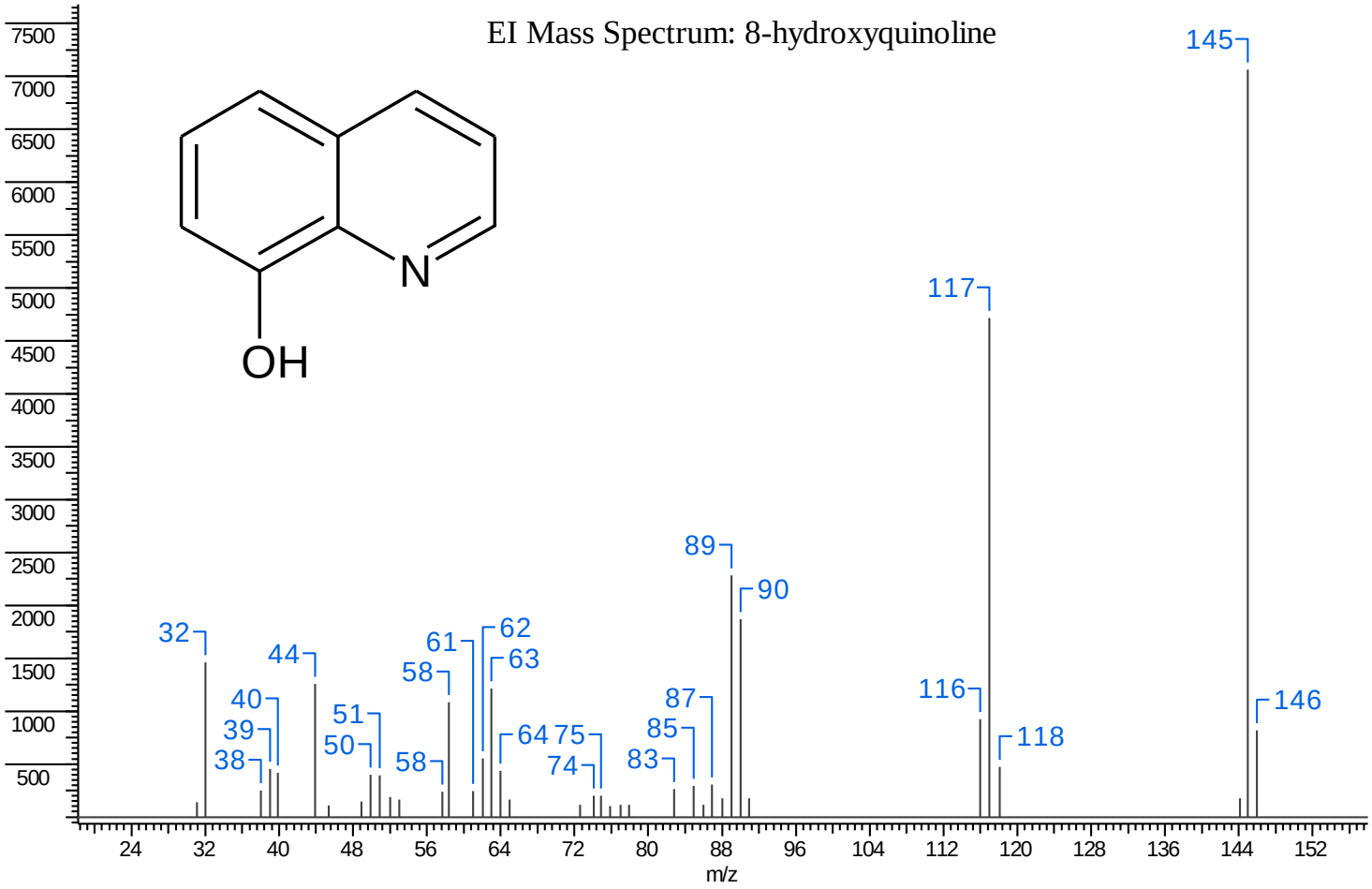
URB597


Abundance
O
NH2
OH
213.1
197.0
139.1
115.1
169.1
63.0
44.0
89.0
154.0
183.0
m / z -->

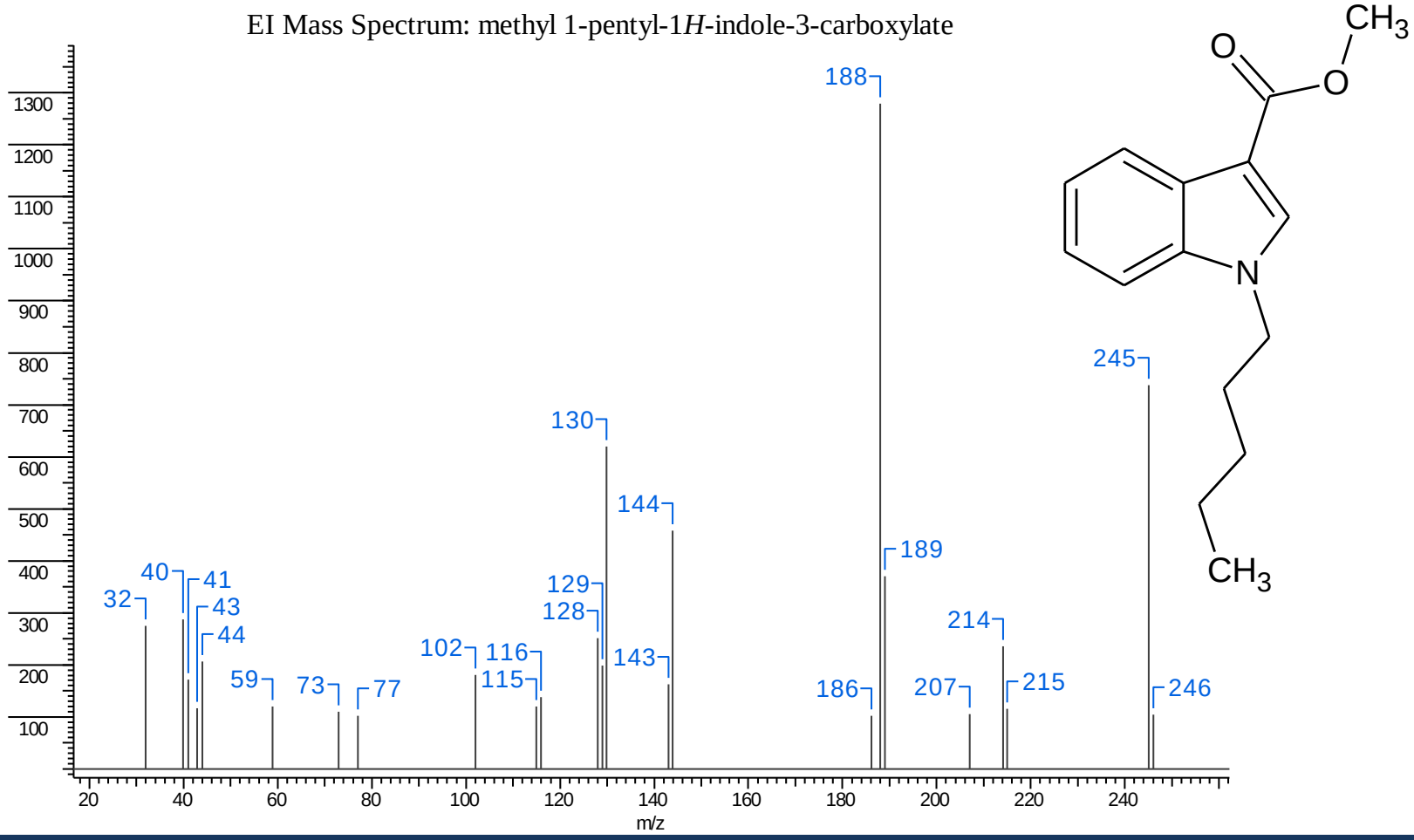
What we can learn: PB-22



What we can learn: PB-22



What we can learn: PB-22



Thank You

Questions????

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